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Buffer and backfill process report for the safety assessment SR-Can

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Preface

This document compiles information on processes in the buffer and deposition tunnel backfill relevant for long-term safety of a KBS-3 repository. It supports the safety assessment SR-Can, which is a preparatory step for a safety assessment that will support the licence application for a final repository in Sweden.

Patrik Sellin, SKB has compiled the report.

Most of the material in the report was contributed by selected experts in the field, in particular Ola Karnland and Lennart Börgesson, Clay Technology AB. See Section 1.2 for a complete list of contributors. The sub-sections describing the handling in the safety assessment of the various processes were written by Patrik Sellin, SKB and the undersigned in collaboration with the concerned experts.

This report has been reviewed in two stages; an early version was review by Roland Pusch, Geodevelopment AB and a later version by David Dixon, AECL and Paul Wersin, Nagra.

Stockholm, October 2006

Allan Hedin

Project leader, SR-Can

Contents

1 Introduction

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

1.1.1 Overall methodology

This report documents buffer and backfill processes identified as relevant to the long-term safety of a KBS-3 repository, and forms an important part of the reporting of the safety assessment SR-Can. The detailed assessment methodology, including the role of the process report in the assessment, is described in the SR-Can Main report, /SKB 2006a/. The following excerpts describe the methodology, and clarify the role of this process report in the assessment.

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

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

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

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

   This step consists of identifying all the factors that need to be included in the analysis. Experience from earlier safety assessments and KBS-3 specific and international databases of relevant features, events and processes (FEPs) influencing long-term safety are utilised. An SKB FEP database is developed where the great majority of FEPs are classified as being either initial state FEPs, internal processes or external FEPs. Remaining FEPs are either related to assessment methodology in general or deemed irrelevant for the KBS-3 concept. Based on the results of the FEP processing, an SR-Can FEP catalogue, containing FEPs to be handled in SR-Can, has been established. This step is documented in the SR-Can FEP report /SKB 2006b/.

2. Description of the initial state.

   The initial state of the system is described based on the design specifications of the KBS-3 repository, a descriptive model of the repository site and a site-specific layout of the repository. The initial state of the fuel and the engineered components is that immediately after deposition, as described in the SR-Can Initial state report /SKB 2006c/. The initial state of the geosphere and the biosphere is that of the natural system prior to excavation, as described in the site descriptive models /SKB 2005ab/. The repository layouts adapted to the sites are provided in underground design reports for each site /Brantberger et al. 2006, Janson et al. 2006/.

3. Description of external conditions.

   Factors related to external conditions are handled in the categories “climate related issues”, “large-scale geological processes and effects” and “future human actions”. The handling of climate related issues is described in the SR-Can Climate report /SKB 2006d/, whereas the few external, large-scale geosphere processes are addressed here in the Geosphere process report. The treatment of future human actions in SR-Can is described in the SR-Can FHA report /SKB 2006e/.

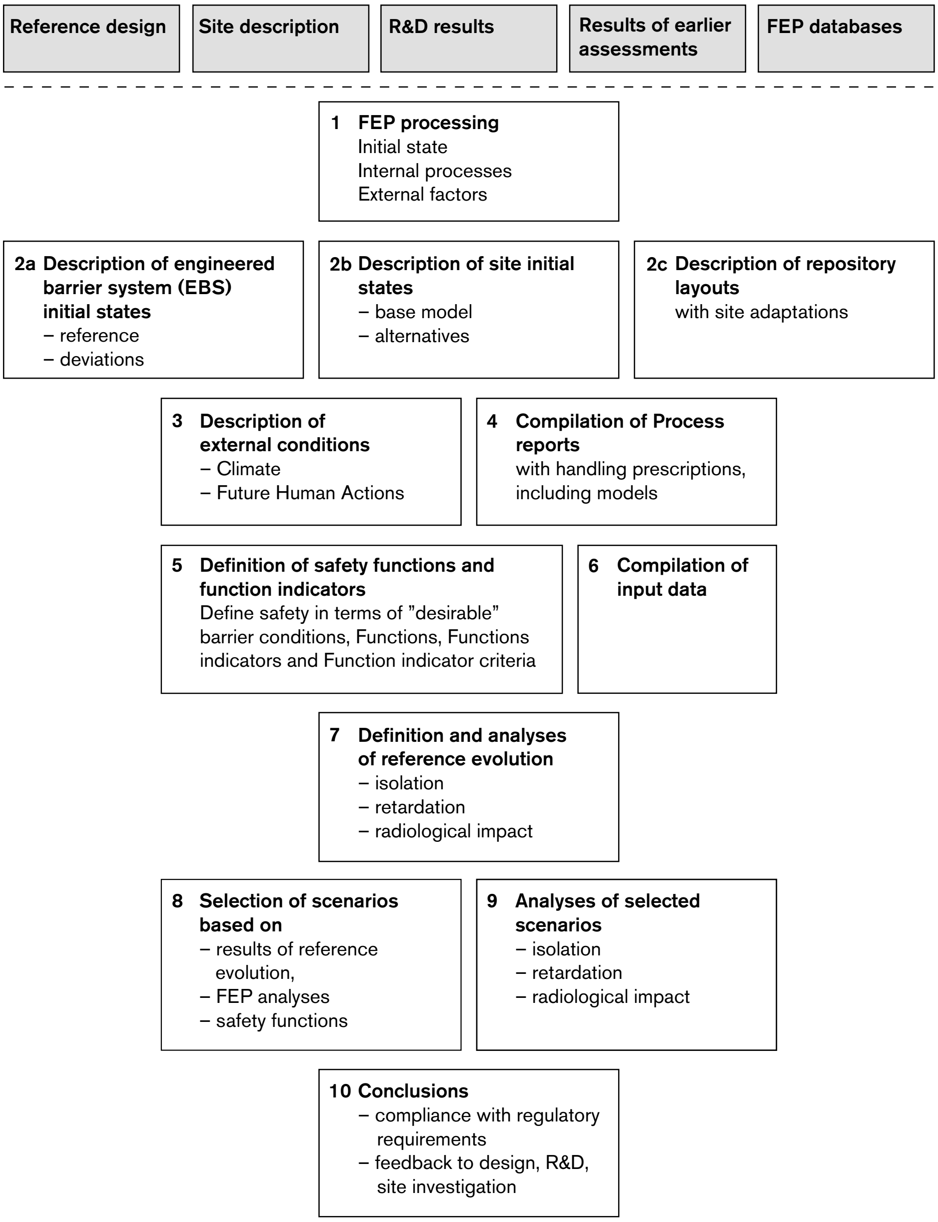


Figure 1-1. *An outline of the ten main steps of the SR-Can safety assessment. The boxes at the top above the dashed line are inputs to the assessment.*

4. Description of processes.

   The identification of relevant processes is based on earlier assessments and FEP screening. All identified processes within the system boundary relevant to the long-term evolution of the system are described in dedicated Process reports, i.e. this report and process reports for the fuel and canister /SKB 2006f/ and for the geosphere /SKB 2006g/. For each process, its general characteristics, the time frame in which it is important, the other processes to which it is coupled and how the process is handled in the safety assessment are documented.

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

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

6. Input data selection.

   Data to be used in the quantification of repository evolution and in dose calculations are selected using a structured procedure. The process of selection and the data adopted are reported in a dedicated Data report /SKB 2006h/. Also, a template for discussion of input data uncertainties has been developed and applied.

7. Definition and analysis of reference evolution.

   A reference evolution, providing a description of a plausible evolution of the repository system, is defined and analysed. The isolating potential of the system over time is analysed in a first step, yielding a description of the general system evolution and an evaluation of the safety function indicators. If the evolution indicates breaching of isolation, the retarding potential of the repository and its environs is analysed and dose consequences are calculated for the long-term conditions identified in the first step. Also, some canister failure modes not resulting from the reference evolution are analysed in order to further elucidate the retarding properties of the system. Each process is handled in accordance with the plans outlined in the process reports.

8. Selection of scenarios.

   A set of scenarios for the assessment is selected. A comprehensive main scenario is defined in accordance with SKI's regulations SKIFS 2002:1. The main scenario is closely related to the reference evolution analysed in step 7. The selection of additional scenarios is focused on the safety functions of the repository and the safety function indicators defined in step 4 form an important basis for the selection. For each safety function, an assessment is made as to whether any reasonable situation where it is not maintained can be identified. If this is the case, the corresponding scenario is included in the risk evaluation for the repository, with the overall risk determined by a summation over such scenarios. The set of selected scenarios also includes e.g. scenarios explicitly mentioned in applicable regulations, such as human intrusion scenarios, and scenarios and variants to explore design issues and the roles of various components in the repository.

9. Analysis of scenarios.

   The main scenario is analysed essentially by referring to the reference evolution in step 7. An important result is a calculated risk contribution from the main scenario. The additional scenarios are analysed by focussing on the factors potentially leading to situations in which the safety function in question is not maintained. In most cases, these analyses are carried out by comparison with the evolution for the main scenario, meaning that they only encompass aspects of repository evolution for which the scenario in question differs from the main scenario. For these scenarios, as for the main scenario, a risk contribution is estimated.

10. Conclusions.

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

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

1.1.2 Identification of processes

The process documentation in the SR 97 version of the Process report /SKB 1999/ is a starting point for this SR-Can version. As a result of the FEP processing (step 1 above), the list of relevant processes has been reviewed and slightly extended, see the SR-Can FEP report /SKB 2006b/ for details. Furthermore, the SR 97 process report covering fuel, canister, buffer/backfill and geosphere processes has been replaced by several reports of which the present one covers geosphere processes. A complete list of processes described in the SR-Can process reports can be found in the abovementioned FEP report.

1.1.3 Intended audience of this report

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

1.2 Structure for process descriptions

All identified processes are documented using the following template, where many of the headings are the same as those used in the SR 97 report:

Overview/general description

Under this heading, a general description of the knowledge regarding the process will be given. For most processes, a basis for this will be the contents of the SR 97 Process report /SKB 1999/. All that text will however be reviewed and updated as necessary.

A table is produced, documenting how the process is influenced by the specified set of physical variables in the relevant system component and how the process influences the variables.

Boundary conditions

The boundary conditions for each process will be discussed. These refer to the boundaries of the relevant system components. For example, for buffer processes the boundaries are the buffer interfaces with the canister, the walls of the deposition hole and the backfill. The processes for which boundary conditions need to be described are, in general, related to transport of material or energy across the boundaries. For example for chemical processes occurring within a system component, like illitisation in the buffer, the discussion of boundary conditions will relate to the boundary conditions of the relevant transport processes occurring in the buffer, i.e. advection and diffusion.

Model studies/experimental studies

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

Natural analogues/observations in nature

If relevant, natural analogues and/or observations in nature regarding the process will be documented under this heading.

Time perspective

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

Handling in the safety assessment SR-Can

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

- defined as irrelevant on the basis of the information under the previous headings,
- defined as irrelevant provided that a certain condition is fulfilled, e.g. that the buffer density is within a certain range,
- included by means of modelling.

The following aspects need to be covered, although no prescribed format for the documentation is given:

Time periods: Over what time period is the process relevant for the system evolution? For example: in the case of the buffer, relevant time periods might be

- the resaturation phase extending from the time of deposition until the point in time when the buffer is fully water saturated,
- the so called thermal phase extending from the time of deposition and throughout the approximately 1,000 year time period of elevated temperature in the buffer or
- the long-term, extending throughout the one million year assessment time and including the varying conditions in the bedrock caused by long-term climate and other environmental variations.

By documenting the relevance of the process for applicable time periods, the process system can be simplified by omitting the process in time periods during which it is not relevant.

Boundary conditions: How are the boundary conditions handled? For example, are spatially and temporally varying chemical and hydraulic conditions considered?

Influences and couplings to other processes: The handling of the documented influences will be discussed, as will couplings to other processes within the system component.

The special cases of failed canister and of earthquakes altering deposition hole or tunnel geometry: These special cases imply altered conditions that could influence many processes in particular for the fuel, the canister, the buffer and the backfill and they may need to be discussed separately. Canister failures and earthquakes of a magnitude that could affect the deposition hole or tunnel geometry are not expected for several thousands of years after deposition when temperate conditions are likely to prevail, meaning that the special cases are not relevant for many "early" processes. Should the assumptions regarding the lack of occurrence of significant, early canister failures or earthquakes not be corroborated by more detailed and integrated analyses in the safety assessment, this simplification of the handling of the special cases will be reconsidered.

As a result of the information under this subheading, a mapping of all processes to method of treatment and, in relevant cases, applicable models will be produced, see the Interim main report /SKB 2004a/ or the main SR-Can report for an example. The mapping will be characterised on different timescales.

Handling of uncertainties in SR-Can

Given the adopted handling in the safety assessment SR-Can as described above, the handling of different types of uncertainties associated with the process will be summarised.

Uncertainties in mechanistic understanding: The uncertainty in the general understanding of the process will be discussed based on the available documentation and with the aim of answering the question: Are the basic scientific mechanisms governing the process understood to a level necessary for the suggested handling? Alternative models may sometimes be used to illustrate this type of uncertainty.

Model simplification uncertainties: 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 uncertainties: The set of input data necessary to quantify the process for the suggested handling will be documented. The further treatment of important input data and input data uncertainties will, at later stages of the SR-Can project, be described in an Input data report, to which reference will be made if relevant.

References

A list of references used in the process documentation.

1.3 Documentation of participating experts and of decisions made

The experts involved in assembling the basic information about the processes are listed in Table 1-1. The sub-sections "Handling in the safety assessment SR-Can" and "Handling of uncertainties in SR-Can" have been produced by Patrik Sellin and Allan Hedin, SKB in collaboration with the expert that assembled the information on the process in question.

In addition, each process description contains a documentation of which expert(s) assembled the basic information on the process, which expert(s) were involved in the decision regarding treatment in the safety assessment and the dates for the final revision of the text and for the final decision on handling to be included. All these experts are included in the SR-Can expert database, see further the SR-Can main report /SKB 2006a/.

1.4 Initial state of the buffer in SR-Can

The following is an overview description of the initial state of the buffer, i.e. its state at the time of deposition. A more formal and exhaustive account is given in the SR-Can initial state report /SKB 2006c/. In that description, the specified set of variables describing the buffer, see Section 1.5, is utilised.

In the deposition hole, the copper canister is surrounded by a buffer of clay. The buffer is installed as bentonite blocks and rings. The blocks are placed below and above the canister and the bentonite rings surround the canister.

Two different types of bentonite are considered as reference buffer material for the purpose of SR-Can. One is a natural Na-bentonite of Wyoming type (MX-80) supplied by the American Colloid Company and the other is Calziumbentonit IBECO DEPONIT CA-N, a natural Ca-bentonite from the Milos island, Greece supplied by Silver and Baryte (non-converted Milos-bentonite). These bentonites consist mainly of the smectite mineral montmorillonite (about 85%) with the characteristic property that it swells when unconfined and in contact with water. The montmorillonite content is not expected to vary by more than a few percent. For an actual repository there may be many possible choices for a suitable buffer material.

Table 1-1. Experts responsible for the documentation of buffer and backfill processes.

Process	Expert author, affiliation
Radiation attenuation/heat generation	Allan Hedin, SKB
Heat transport	Harald Hökmark, Clay Technology
Freezing	Sven Knutsson, Luleå University of Technology, Lennart Börgesson, Clay Technology
Water uptake and transport under unsaturated conditions	Lennart Börgesson, Clay Technology
Water transport under saturated conditions	Lennart Börgesson, Ola Karnland, Clay Technology
Gas transport/dissolution	Patrik Sellin, SKB
Piping/erosion	Lennart Börgesson, Clay Technology
Swelling/mass redistribution	Lennart Börgesson, Clay Technology
Liquefaction	Lennart Börgesson, Clay Technology
Advection	Ola Karnland, Clay Technology
Diffusion	Michael Ochs, BMG Engineering
Colloid transport	Patrik Sellin, SKB
Sorption (including ion exchange)	Michael Ochs, BMG Engineering
Alterations of impurities	Jordi Bruno, David Arcos, Enviros, Patrik Sellin SKB
Aqueous speciation and reactions	Patrik Sellin, SKB
Osmosis	Ola Karnland, Clay Technology
Montmorillonite transformation	Ola Karnland, Clay Technology
Colloid release	Ola Karnland, Clay Technology
Radiation-induced transformations	Patrik Sellin, SKB
Radiolysis of pore water	Lars Werme, SKB
Microbial processes	Karsten Pedersen, University of Göteborg, Ola Karnland, Clay Technology
Speciation of radionuclides	Patrik Sellin, SKB
Transport of radionuclides in water phase	Patrik Sellin, SKB
Transport of RN in gas phase	Patrik Sellin, SKB

MX-80 contains in addition to smectite other accessory minerals: albite, quartz, cristobalite, muscovite and gypsum, and in addition, grains of pyrite, calcite, siderite, barite and iron hydroxides (see Table 1-2). The mean chemical compositions, as analysed by ICP/AES, of MX-80 expressed as oxides is: 57% SiO_2, 18.5% Al_2O_3, 3.6% Fe_2O_3, 2.3% MgO, 1.3% CaO, 2.0% Na_2O, 0.5% K_2O, 0.2% TiO_2, 0.3% total carbon, 0.3% total sulfur, and 13.7% loss of ignition.

Other minerals in Milos-bentonite are mainly calcite, dolomite, quartz, and cristobalite, see Table 1-2. The mean chemical compositions, expressed as oxides as analysed by ICP/AES, of the two bentonites are 48% SiO_2, 15.7% Al_2O_3, 4.56% Fe_2O_3, 2.92% MgO, 5.4% CaO, 0.7% Na_2O, 0.8% K_2O, 0.7% TiO_2, 1.0% total carbon, 0.7% total sulfur, and 20% loss of ignition.

There are primarily two methods available for fabrication of bentonite blocks and rings; unaxial pressing and isostatic pressing. Objects thicker than 0.5–1 m cannot be easily produced by unaxial pressing and the development of isostatic pressing is therefore important, since no equipment to fabricate full size buffer components with isostatic pressing is available in Sweden today. Fabrication of the blocks and rings by isostatic pressing requires that the objects are machined to the tolerances specified.

The bentonite, bought in bulk form and transported by ship, is subject to quality control both before loading in the ship and at reception. This is done to ensure that the quality is within the specifications and that there is no contamination during the transport. Quality control is undertaken also during the manufacture of the blocks and rings; one important check is the water content before pressing so that this can be adjusted to get the correct water content for the manufacturing process.

The primary goal in the manufacture of bentonite blocks and rings and the subsequent deposition process is to achieve a pre-defined final density in the water-saturated buffer once post-emplacement equilibration has occurred. The currently defined range of density required for the saturated buffer is 1,950–2,050 kg/m^3. The bulk density is dependent on the slots left for technical reasons between the canister and buffer and between buffer and rock. The slot between the canister tube and the buffer is 5 mm wide and the slot along the circumferential boundary between the buffer and the rock is 30 to 50 mm. The slots are either left open or are filled with bentonite pellets. It is still a subject of discussion as to wheather the outer slot should be filled with pellets or not. Gap filling may ultimately be a site specific issue.

The buffer emplacement in the boreholes of each tunnel may take place several months after the deposition holes were drilled. The deposition holes are assumed to have filled with water in the period between drilling and buffer emplacement, which is why draining is the first step in the preparation of the holes. Deposition of buffer and the canister starts at the hole at the outermost end of the tunnel. The buffer is put into position by a specially designed buffer filling vehicle. The bentonite positioning is thereafter checked and possibly adjusted. The emplacement of the copper canister is done with a specially designed deposition machine that also places a top bentonite block immediately after the canister is emplaced. The emplacement of the canister will probably be documented with a photograph of the canister in its final position before the remaining bentonite blocks are emplaced. The final handling procedures and the final design of the buffer filling vehicle and the deposition machine are not decided yet, but do not affect this description of the general work procedures. Small geometric tolerances in the deposition holes mean a small risk for faulty emplacement of the buffer and canister.

The bentonite must be protected from water or high humidity until the tunnel is backfilled. The reason is that the buffer may start swelling before the deposition of the canister and before the tunnel backfilling can apply its counterweight on the buffer. One possible method is to insert a drain tube in the deposition hole and to protect the whole buffer with a plastic bag that is kept sealed until the backfilling of the tunnel starts. The plastic bag and drain tube would be removed after use.

Table 1-2. Impurities and accessory minerals in MX-80 and Deponit CA-N bentonite /Karnland et al. 2006/.

Component	MX-80 (wt-%)	Deponit-CaN (wt-%)	±
Albite	3	0	1
Anorthoclase	0	2	1
Calcite + Siderite	0	10	1
Cristobalite	2	1	0.5
Dolomite	0	3	1
Gypsum + anhydrite	0.7	1.8	0.2
Mica	4	0	1
Montmorillonite	87	81	3
Pyrite	0.07	0.5	0.05
Quartz	3	1	0.5
CEC (meq/100g)	75	70	2
Na^+	72%	24%	5% units
Ca^{2+}	18%	46%	5% units
Mg^{2+}	8%	29%	5% units
K^+	2%	2%	1% units

1.5 Definition of buffer variables

Each component in the EBS initial state is described by a specified set of physical variables, selected to allow an adequate description of the long-term evolution of the component in question in the safety assessment.

The buffer is bounded on the inside by an interface with the canister, on the outside by the interfacewith the rock surface of the deposition hole, at the bottom by an interface with the concrete plate at the base of the borehole and on the top by its interface with the backfill.

The buffer, as it is delimited by the variable buffer geometry, is characterised thermally by its temperature and with respect to radiation by the intensity of the radiation field it is exposed to, mainly γ and neutron radiation.

Hydraulically, the buffer is characterised by its water content, and sometimes by gas concentrations and by hydrovariables (pressure and flows), which are mainly of interest in the phase when the buffer is being saturated with water.

The buffer is mechanically characterised by its stress state.

The chemical state of the buffer is defined by its composition, including the montmorillonite composition, the other clay minerals, and any other impurities. The chemical state is also defined by the pore water composition and the occurrence of structural and stray materials in the deposition hole.

The variables are defined in Table 1-3. The values of some of the variables are dependant on the density of the different phases. The following values have been used: density of water (ρ_w) is 1,000 kg/m^3 and density of clay solids (ρ_{cs}) is 2,780 kg/m^3.

The initial values of the variables, i.e. the values at the time of deposition, are given in the SR-Can initial state report /SKB 2006c/.

Table 1-3. Definition of buffer variables.

Variable	Definition
Buffer geometry	Geometric dimensions for buffer. An example is, description of interfaces (on the inside towards the canister and on the outside towards the geosphere).
Pore geometry	Pore geometry as a function of time and space in buffer. The porosity, (the fraction of the volume that is not occupied by solid material) is often given.
Radiation intensity	Intensity of (α, β,) γ and neutron radiation as a function of time and space in buffer.
Temperature	Temperature as a function of time and space in buffer.
Water content	Water content as a function of time and space in buffer.
Gas content	Gas contents (including any radionuclides) as a function of time and space in buffer.
Hydrovariables (pressure and flows)	Flows and pressures of water and gas as a function of time and space in buffer.
Stress state	Stress conditions as a function of time and space in buffer.
Bentonite composition	Chemical composition of the bentonite (including any radionuclides) in time and space in buffer, levels of impurities in time and space in buffer together with impurities also include minerals, other than smectite.
Montmorillonite composition	The mean molecular structure of the montmorillonite mineral including the type of charge compensation cations
Pore water composition	Composition of the pore water (including any radionuclides and dissolved gases) in time and space in the buffer.
Structural and stray materials	Chemical composition and quantity of concrete bottom in deposition holes.

1.6 Buffer performance and safety

In order to evaluate buffer performance in the safety assessment, a number of so called function indicators and criteria that these should fulfil over time, have been formulated, see further the SR-Can main report, /SKB 2006a/. The criteria are summarised in Table 1-4, where also references to the sections in this report where the criteria are motivated are given.

1.7 Summary of handling in safety assessment

Table 1-5 summarises the handling of buffer processes in the safety assessment SR-Can, as suggested in this report. In the table, the process is either "mapped" to a model by which it will be quantified or associated with a brief verbal description of how it will be handled. Since the initial evolution, characterised by unsaturated conditions and elevated temperatures is in many respects different from the long-term, saturated phase, the description in the table has been divided accordingly.

The information in the table can be summarised as follows:

For the initial saturation phase, the peak canister and buffer temperatures and the THM evolution as the buffer saturates need to be quantified. Modelling of the thermal evolution of the entire near field will be performed with the near field evolution model to evaluate peak canister and buffer temperatures. Coupled THM modelling of the buffer will be performed to clearly describe the hydraulic evolution for different hydraulic conditions in the bedrock. The swelling at the end of the saturation phase is addressed by both the system model and the THM model, where the former can be used for rapid evaluations of the final result of the swelling for a number of input data combinations, including osmosis effects due to intruding saline water and the latter could simulate the pathway to the final result.

The chemical evolution during the thermal phase of elevated and varying temperature in the buffer will be addressed by the chemistry model.

Most other processes are not to any significant extent affected by the thermal and unsaturated conditions and are therefore neglected during the early saturation and thermal phases.

Table 1-4. Summary of the buffer function indicators and the criteria they should fulfil.

Function indicator	Criterion	Rationale	Reference
Bulk hydraulic conductivity	$k^{Buff} < 10^{-12}$ m/s	Limit mass transport to a diffusion dominated process	2.3.2
Swelling pressure	$P_{Swell}^{Buff} > 1$ MPa	Ensure tightness, self sealing,	2.3.2
Maximum temperature	$T^{Buffer} < 100°C$	Ensure that the buffer will retain its favourable properties in a long term perspective	2.5.9
Minimum temperature	$T^{Buffer} > 0°C$	Avoid freezing	2.2.2
Swelling pressure around entire canister	$P_{Swell}^{Buff} > 0.2$ MPa	Avoid canister sinking (criterion to be determined)	2.4.1
Buffer density around entire canister	$\rho_{Bulk}^{Buff} >1,800$ kg/m^3	Exclude microbial activity	2.5.13
Buffer density around entire canister	$\rho_{Bulk}^{Buff} >1,650$ kg/m^3	Prevent colloid transport through buffer	2.5.4
Buffer density around entire canister	$\rho_{Bulk}^{Buff} < 2,100$ kg/m^3	Ensure protection of canister against rock shear	2.4.1

The long-term chemical evolution following the thermal phase will be addressed by both the chemistry model and the system model and for the varying boundary conditions expected as a result of climate change etc. The former model provides a spatially resolved result and involves more chemical reactions whereas the latter can be used for rapid evaluations for a number of input data combinations. Montmorillonite transformation is handled by separate modelling. Erosion due to dilute intruding groundwater during glacial conditions must be addressed if the hydrogeochemical analyses imply that ionic strengths below the given criterion cannot be excluded. Colloidal release needs to be modelled accordingly.

The effects of the chemical evolution on key properties like swelling pressure and hydraulic conductivity will be evaluated using empirical relationships. A number of issues related to mass redistribution in the buffer still need to be evaluated for the long-term evolution.

In the case of a canister failure, the release of gas from the corroding cast iron canister insert will be handled by quantitative estimates based on experimental studies of gas transport through bentonite. Diffusion of radionuclides through the buffer is calculated with radionuclide speciations, necessary for the selection of diffusion and sorption data, estimated on the basis of experimental data. Transport of fuel colloids through the bentonite is neglected if the buffer density exceeds a specified value, otherwise the effect of this process on dose consequences is estimated by a bounding calculation case.

Table 1-5. Process table for the buffer describing how buffer processes are handled in different time frames and for the special case of an earthquake. Green fields denote processes that are neglected or not relevant for the time period of concern. Red fields denote processes that are quantified by modelling in the safety assessment. Orange fields denote processes that are neglected subject to a specified condition.

	Resaturation/ ”thermal” period	Long-term after saturation and “thermal” period	Earthquakes	Notes
Intact canister				
Bu1 Radiation attenuation/heat generation	Neglected since dose rate is too low to be of importance for the buffer.	Neglected since dose rate is too low to be of importance for the buffer.	Not relevant	
Bu2 Heat transport	System model	System model	Not relevant	
Bu3 Freezing	Neglected, since this requires permafrost conditions	Neglected if buffer temperature > −5°C. Otherwise bounding consequence calculation.	Not relevant	Repository temperature in long term obtained from permafrost depth modelling.
Bu4 Water uptake and transport for unsaturated conditions	THM model	Not relevant by definition	Not relevant	
Bu5 Water transport for saturated conditions	Neglected under unsaturated conditions, For saturated conditions the treatment is the same as for “Long-term”	Neglected if hydraulic conductivity < 10^{-12} m/s since diffusion would then dominate	Consider pressure transients	The consequences of a buffer with high hydraulic conductivity are evaluated. Two different cases are studied: the buffer acts as a porous medium with high conductivity (mass loss) the buffer is fractured (alteration)

	Resaturation/ ”thermal” period	**Long-term after saturation and “thermal” period**	**Earthquakes**	**Notes**
Bu6 Gas transport/ dissolution	Through dissolution	(Through dissolution) No gas phase is assumed to be present	(Through dissolution) No gas phase is assumed to be present	
Bu7 Piping/erosion	Model study	Not relevant, see also Bu17	Not relevant	Loss of buffer mass is calculated
Bu8 Swelling/Mass redistribution	THM modelling including interaction buffer/backfill and thermal expansion System model (final swelling)	Integrated evaluation of erosion, convergence, corrosion products, creep, swelling pressure changes due to ion exchange and salinity, canister sinking	Part of integrated assessment of buffer/canister/ rock	Need to also consider deviations in amount of buffer initially deposited.
Bu9 Liquefaction	Not relevant	Neglected	Neglected since liquefaction from a short pulse cannot occur in a high density bentonite, due to high effective stresses.	
Bu10 Advection	Simplified assumptions of mass transport of dissolved species during saturation.	Neglected if hydraulic conductivity $< 10^{-12}$ m/s	Consider pressure transients	See “Water transport for saturated conditions”
Bu11 Diffusion	Chemistry model (thermal, saturated phase; unsaturated phase disregarded)	Chemistry model	Consider altered geometry (diffusion pathways).	Consider varying groundwater compositions The initial thermal gradient is considered
Bu12 Sorption (including ion-exchange)	Chemistry model (thermal, saturated phase; unsaturated phase disregarded)	Chemistry model		
Bu13 Alterations of impurities	Chemistry model (thermal, saturated phase; unsaturated phase disregarded)	Chemistry model		
Bu14 Pore water speciation	Chemistry model (thermal, saturated phase; unsaturated phase disregarded)	Chemistry model		
Bu15 Osmosis	System model (initial swelling)	Evaluation through comparison with empirical data System model		Handling of long-term intrusion of saline water
Bu16 Montmorillonite transformation	Model calculations (thermal, saturated phase; unsaturated phase disregarded)	Model calculations		
Bu17 Colloid release	Neglected if $[M^{2+}] > 1$ mM Otherwise modelled	Neglected if $[M^{2+}] > 1$ mM Otherwise modelled		Loss of buffer mass is calculated See also water transport under saturated conditions

	Resaturation/ ”thermal” period	**Long-term after saturation and “thermal” period**	**Earthquakes**	**Notes**
Bu18 Radiation-induced transformations	Neglected since dose rate outside canister is too low to have any effect	Neglected since dose rate outside canister is too low to have any effect		
Bu19 Radiolysis of pore water	Neglected since dose rate outside canister is too low to have any effect	Neglected since dose rate outside canister is too low to have any effect		
Bu20 Microbial processes	Neglected under unsaturated conditions, since the extent of aqueous reactions is limited. For saturated conditions the treatment is the same as for “Long-term”	Neglected if swelling pressure > 2 MPa, otherwise quantitative estimate of sulphate reduction		
Failed canister				
Bu6 Failed canister. Gas transport/ dissolution	Quantitative estimate based on empirical data *(no failures are expected this period)*	Quantitative estimate based on empirical data		
Bu18 Failed canister. Radiation-induced transformations	Neglected since dose rate outside canister is too low to have any effect	The effect of α-radiation from nuclides from a failed canister is estimated		The effect of α-radiation from nuclides is estimated in the section 2.5.11. There, it is concluded that the consequences can be neglected.
Bu21 Colloid transport	Neglected if density at saturation > 1,650 kg/m^3, otherwise bounding calculation *(no failures are expected this period)*	Neglected if density at saturation > 1,650 kg/m^3, otherwise bounding calculation		
Bu22 Speciation of radionuclides	Assumptions based on empirical data *(no failures are expected this period)*	Assumptions based on empirical data		
Bu23 Transport of radionuclides in water phase	COMP23 Analytic *(no failures are expected this period)*	COMP23 Analytic		
Bu24 Transport of radionuclides in gas phase	Quantitative estimate *(no failures are expected this period)*	Quantitative estimate		

1.8 Initial state of the backfill in SR-Can

The following is an overview description of the initial state of the backfill, i.e. its state at the time of deposition. A more formal and exhaustive account is given in the SR-Can Initial state report /SKB 2006c/. In that description, the specified set of variables describing the backfill, is utilised.

When the holes in a deposition tunnel have been filled with canisters and the buffer the tunnel will be backfilled. Before backfilling, all tunnel installations including concrete on the floor of the tunnel will be removed.

Two backfill concepts will be analysed in SR-Can:

- Precompacted blocks of a natural swelling clay (not necessarily a bentonite), Friedland clay is used as an example of such a material in SR-Can. The whole tunnel is filled with pre-compacted blocks. The gaps between the rock and the blocks are filled with pellets of the same material. The estimated volumes and proposed densities are given in Table 1-6.
- Precompacted blocks made of a mixture of bentonite of buffer quality and crushed rock with a weight ratio of 30/70. The gaps between the rock and the blocks are filled with bentonite pellets. The maximum grain size for the ballast material (the crushed rock) is recommended to will be 5 mm. The volumes and densities for the mixture are given in Table 1-7.

Friedland Clay is a natural clay, which mainly consists of mixed layer smectite/illite. The full composition is given in Table 1-8, and the mean chemical composition, expressed as oxides as analysed by ICP/AES, of the two bentonites is: 61% SiO_2, 17.3% Al_2O_3, 6.4% Fe_2O_3, 1.9% MgO, 0.4% CaO, 1.1% Na_2O, 3.1% K_2O, 0.9% TiO_2, 0.6% total carbon, 0.5% total sulfur, and 7.6% loss of ignition.

The bentonite component in the 30/70 mixture is assumed to have the same composition as the buffer bentonite. The compositions are given in Table 1-2. The crushed rock is taken from the residues from the excavation of the repository.

Table 1-6. Volumes and densities for Friedland Clay.

Material	Estimated fraction of tunnel area (%)	Dry density kg/m^3
Block	78	2,000
Pellets	20	1,100
Void	2	0

Table 1-7. Volumes and densities for 30/70 blocks and pellets.

Material	Estimated fraction of tunnel area (%)	Dry density kg/m^3	Effective dry clay density[1] (kg/m^3)
Block	78	2,190	1,559
Pellets	20	1,100	1,100
Void	2	0	0
Average	100	1,928	1,335

---

[1] The effective clay dry density (ECDD) is defined as the mass of the clay component divided by the volume occupied by bentonite clay and voids. The volume occupied by nonbentonite materials is considered to be an inert filler /Dixon et al. 2002/. The ECDD concept is convenient to use for comparison of a specific bentonite mixed with other materials such as sand or crushed rock. The effective dry montmorillonite density (EMDD) is defined as the mass of the montmorillonite component divided by the volume of the montmorillonite component and voids. The EMDD may be used also for comparison between different bentonites, assuming that the montmorillonite components are relatively similar, since also the accessory minerals are considered to be an inert filler.

Table 1-8. Mineralogical composition of Friedland Clay /Karnland et al. 2006/.

Component	Friedland (wt-%)	±	
Feldspars	3	1	
Gypsum	0.8		From chemical analysis
Illite	4	2	
Kaolin	10	5	
Mica (muscovite)	9	5	
Mixed layer clay	44	5	33% non-expandable, 67% expandable layers
C organic	0.6		From chemical analysis
Pyrite	0.62		From chemical analysis
Quartz	28	3	
CEC (meq/100g)	22	2	

1.9 Definition of backfill variables

The deposition tunnel is constrained by the rock surrounding the tunnel but also by the buffer in the deposition holes and the plugs at the tunnel ends. In the case of rejected deposition holes /SKB 2006c/, the subsystem is constrained also by the rock around rejected deposition holes.

The backfill in the deposition tunnel as it is delimited by the variable backfill geometry is characterised thermally by its temperature. Hydraulically it is characterised by its pore geometry, water content, gas content and the hydrovariables (pressure and flow). Mechanically, the backfill is characterised by the stress state. The chemical state of the backfill is defined by the material composition. The chemical state is also defined by the pore water composition and the occurrence of structural and stray materials in the deposition hole.

The radiation intensity (dose rate) in the backfill has not been calculated, since it is considerably lower than on the outside of the buffer and is of no importance in the safety assessment.

All variables are defined in Table 1-9.

The initial values of the variables are given in the SR-Can Initial State Report /SKB 2006c/.

1.10 Backfill performance

In order to evaluate the performance of the tunnel backfill, a few so called function indicators and criteria these should fulfil over time, have been established, see further the SR-Can main report. These criteria are summarised in Table 1-10 where references to the sections in this report where the reasoning for these criteria are given.

Table 1-11 summaries the handling of backfill processes in the safety assessment SR-Can, as suggested in this report. In the table, the process is either “mapped” to a model by which it will be quantified or associated with a brief verbal description of how it will be handled. Since the initial evolution, characterised by unsaturated conditions and elevated temperatures is in many respects different from the long-term, saturated phase, the description in the table has been divided accordingly.

Table 1-9. Variables for the tunnel backfill.

Variable	Definition
Backfill geometry	Geometric dimensions for backfill. A description of e.g. interfaces towards buffer and towards the geosphere.
Backfill pore geometry	Pore geometry as a function of time and space in backfill. The porosity, i.e. the fraction of the volume that is not occupied by solid material is often given.
Temperature	Temperature as a function of time and space in deposition tunnels.
Water content	Water content as a function of time and space in deposition tunnels.
Gas content	Gas contents (including any radionuclides) as a function of time and space in deposition tunnels.
Hydrovariables (pressure and flows)	Flows and pressures of water and gas as a function of time and space in deposition tunnels.
Stress state	Stress state as a function of time and space in backfill.
Backfill materials – composition and content	Chemical composition and content of the backfill (including any radionuclides) in time and space. This variable also includes material sorbed to the surface.
Backfill pore water composition	Composition of the pore water (including any radionuclides and dissolved gases) in time and space in backfill.
Structural and stray materials	Chemical composition and quantity of structural materials (rock bolts, filling material in boreholes for grouting, nets etc.) and stray materials in deposition tunnels.

Table 1-10. Summary of the Tunnel Backfill function indicators and the criteria they should fulfil.

Function indicator	Criterion	Rationale	Reference
Bulk hydraulic conductivity	$k^{Backfill} < 10^{-10}$ m/s	Limit advective transport	3.2.2
Swelling pressure	$P_{Swell}^{Backfill} > 0.1$ MPa	Ensure homogeneity	3.2.2
Minimum temperature	$T^{Backfill} > 0°C$	Avoid freezing	3.1.2

The information in the table can be summarised as follows:

- For the initial saturation phase, the saturation and swelling of the backfill and its interaction with the buffer needs to be quantified.
- If hydraulic gradients are present in the early phase, the potential effect of piping and erosion has to be evaluated.
- The temperature increase in the backfill will be moderate and therefore no effects of elevated temperature will be evaluated.

The most important processes in the long-term are physical and chemical processes that could lead to an undesired change of backfill properties. These include ion-exchange, osmosis, colloid release and montmorillonite transformation.

In the case of a canister failure, radionuclide transport in the backfill will be calculated both in the near- and far field models, including advective and diffusive transport as well as sorption.

Table 1-11. Process table for the backfill describing how backfill processes will be handled in different time frames and in the special cases of earth quakes and failed canisters. (Green fields denote processes that are neglected or irrelevant for the time period of concern. Red fields denote processes that are quantified by modelling in the safety assessment. Orange fields denote processes that are neglected subject to a specified condition.)

	Resaturation/ ”thermal” period	**Long-term after saturation and “thermal” period**	**Notes**
Intact canister			
BfT1 Heat transport	Simplified assumption	Simplified assumption	
BfT2 Freezing	Neglected, since this requires permafrost conditions.	Neglected if backfill temperature > 0°C. Otherwise bounding consequence calculation. Note that only deposition tunnels are considered in SR-Can.	Less severe consequences than for buffer.
BfT3 Water uptake and transport for unsaturated conditions	THM model	Not relevant by definition	The pellets are included in the model
BfT4 Water transport for saturated conditions	Neglected under unsaturated conditions, for saturated conditions the treatment is the same as for “Long-term”	Included in geosphere modelling.	Evaluate effects on conductivity of chemical evolution and mass redistribution/loss and of possible changes of hydraulic gradients for permafrost and glaciation
BfT5 Gas transport/ dissolution	THM model	(Through dissolution)	The presence of a trapped gas phase is considered in the modelling of the saturation of the backfill (not the case for the buffer)
BfT6 Piping/erosion	Model study	Not relevant, see also BfT16	See also water transport for saturated conditions
BfT7 Swelling/Mass redistribution	THM modelling including interaction buffer/backfill and homogenisation in tunnel. System model (final swelling)?	Integrated evaluation of erosion, convergence, creep, swelling pressure changes due to ion exchange and salinity and transformation	Need to also consider deviations in amount of buffer and backfill initially deposited and buffer saturating before tunnel backfill.
BfT8 Liquefaction	Not relevant	Not relevant	Less severe consequences than for buffer.
BfT9 Advection	Simplified assumptions of mass transport of dissolved species during saturation.	Included in geosphere modelling.	See “Water transport for saturated conditions”
BfT10 Diffusion	The early stage is not studied specifically, since the conditions in the backfill will be about the same as for the long-term evolution	Chemistry model System model?	Consider varying groundwater composition
BfT11 Sorption (including ion-exchange)	The early stage is not studied specifically, since the conditions in the backfill will be about the same as for the long-term evolution	Chemistry model System model?	Ion-exchange data for Friedland is missing. See also osmosis

	Resaturation/ ”thermal” period	**Long-term after saturation and “thermal” period**	**Notes**
BfT12 Alterations of impurities	The effect on inorganic reduction of oxygen is modelled	Chemistry model System model?	
BfT13 Pore water speciation	The early stage is not studied specifically, since the conditions in the backfill will be about the same as for the long-term evolution	Chemistry model	
BfT14 Osmosis	Hydraulic conductivity in THM model chosen so as to handle osmosis	Evaluation through comparison with empirical data	Handling of long-term intrusion of saline water
BfT15 Montmorillonite transformation	Model calculations (thermal, saturated phase; unsaturated phase disregarded)	Model calculations	
BfT16 Colloid release	Neglected if $[M^{2+}] > 1$ mM Otherwise modelled	Neglected if $[M^{2+}] > 1$ mM Otherwise modelled	Loss of backfill is calculated
BfT17 Radiation-induced transformations	Neglected, since dose rate in backfill is too low to have any effect	Neglected, since dose rate in backfill is too low to have any effect	
BfT18 Microbial processes	Excluded, (the effect on oxygen consumption is not considered)	Excluded at this stage	
Failed canister			
BfT5 Failed can. Gas transport/ dissolution	Neglected, since gas volumes (from buffer) assumed to be too low to reach backfill during this period	Neglected, pessimistically since transport would delay radioactive releases and decrease buffer pressure. The backfill would act as a sink for gas.	Gas release from canister
BfT19 Colloid formation and transport	See geosphere (no failures are expected this period)	See geosphere	Called “colloid transport” for buffer Reference to corresponding geosphere process
BfT20 Speciation of radionuclides	*Assumptions based on empirical data (no failures are expected this period)*	*Assumptions based on empirical data*	
BfT21 Transport of radionuclides in water phase	*COMP23* *Analytic (no failures are expected this period)*	*COMP23* *Analytic*	
BfT22 Transport of radionuclides in gas phase	*By-passed (no failures are expected this period)*	*By-passed*	

2 Buffer processes

2.1 Radiation-related processes

2.1.1 Radiation attenuation/heat generation

Overview/general description

Gamma and neutron radiation from the canister are attenuated in the buffer. The process is described in /SKB 2006f/ The maximum dose outside the canister has been calculated to be less than 500 mGy/h. The dose is dominated by Cs-137, which has a half life of ~ 30 years. The radiation that is not attenuated reaches out into the near-field rock. The main part of the gamma radiation from the spent fuel gets shielded by the iron and copper in the canister. Only a minor fraction ever reached the buffer.

The radiation is of importance for the chemical processes radiation-induced montmorillonite decomposition and gamma radiolysis of pore water.

Table 2-1 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Table 2-1. Process/variable table for the process Radiation attenuation/heat generation.

Variable	Does this variable influence the process?		Does the process influence this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Buffer geometry	Yes	Included in dose rate calculation	No	
Pore geometry	No		No	
Radiation intensity	Yes	Included in dose rate calculation	Yes	Included in dose rate calculation
Temperature	No		Yes	Neglected since it is negligible compared to other processes influencing temperature
Water content	Yes	Included in dose rate calculation	No	
Gas content	Yes	Included in dose rate calculation	No	
Hydrovariables (pressure and flows)	No		No	
Stress state	No		No	
Bentonite composition	Yes	Included in dose rate calculation	No	
Montmorillonite composition	Yes	Included in dose rate calculation	yes	Negligible, see 2.5.11
Pore water composition	Negligible		No	
Structural and stray materials	No		Negligible	Of no concern

The result is a radiation field in the buffer that can lead to radiolysis and that has a marginal impact on the montmorillonite, see further Section 2.5.11.

Attenuation of gamma and neutron radiation will raise the temperature of the buffer, but the effect is negligible compared with other temperature-raising processes.

Boundary conditions

The boundary condition is the radiation intensity to which the buffer is exposed, i.e. the flux leaving the canister outer surface.

Model studies/experimental studies

Attenuation of gamma and neutron radiation can be calculated theoretically for an arbitrary material if geometry and composition are known, see e.g. the model studies mentioned for the corresponding process in the canister. Experimental studies of radiation attenuation in bentonite are reported in Section 2.5.11.

Natural analogues/observations in nature

Not applicable.

Time perspective

The time perspective is determined by the decay properties of the spent fuel. The gamma and neutron radiation is significant during approximately 1,000 years. See further /Håkansson 1999/ for details of the fuel decay characteristics.

Handling in the safety assessment SR-Can

Quantification of this process is needed to evaluate the processes 2.5.11 Radiation-induced transformations and 2.5.12 Radiolysis of pore water. The former is shown to be negligible in Section 2.5.11, for the relevant radiation intensities. The latter could affect the canister surface, but also this effect is shown to be insignificant, see further Sections 2.5.12 and the relevant canister process The radiation field outside canister has been calculated in /Lungren 2004/. The calculated dose rate is ~ 500 mGy/h at deposition.

Time periods: The gamma and neutron radiation is significant during approximately 1,000 years.

Boundary conditions: The radiation flux leaving the canister outer surface is described qantified.

Influences and couplings to other processes: The geometry and the material compositions influence this process. Simple bounds can be put on the effects of temporal variations of the material compositions.

The special cases of failed canister and of earthquake: Canister failures and earthquakes of a magnitude that could affect the process are not expected during the roughly 1,000 year time period in which there is any significant radiation. The process is thus not handled for these cases. Should the assumptions regarding significant, early canister failures or earth quakes not be confirmed by the results of the safety assessment, the handling of the special cases will be reconsidered.

Uncertainties

Uncertainties in mechanistic understanding

The understanding of the process is deemed sufficient for the needs of the safety assessment.

Model simplification uncertainties for the above handling in SR-Can

Not relevant.

Input data and data uncertainties for the above handling in SR-Can

In general, data for a quantitative description of the process are known with sufficient accuracy for the needs of the safety assessment, considering the small effects of this process on the repository system.

2.2 Thermal processes

2.2.1 Heat transport

Overview/general description

Heat is transported from the canister surface to the buffer, through the buffer and finally from the buffer to the rock both directly and via the tunnel backfill. The first time after deposition there will be gaps between the canister and the buffer and between the buffer and the rock. During this time, heat will be transported by a combination of radiation and conduction across the two gaps and by pure conduction across the bentonite that will be unsaturated. There may be some convection, but because of the low permeability of the bentonite and because of the narrow gap geometries, this contribution can be ignored. In particular the heat resistance of the gap between canister and bentonite will be high because of the low emissivity of the copper surface and the associated low radiant heat transfer. The heat resistance of the gap between buffer and rock will be lower and will not have such an impact on the canister temperature as the canister/buffer gap. In addition, the buffer/rock gap will start to close soon after deposition while the canister/buffer gap will remain open longer. The efficiency of the heat transport through the buffer region is important for the performance of the system, since it affects two important temperatures: that of the canister surface and that in the buffer itself.

When the buffer has been water-saturated and has swelled out so that all gaps and joints are filled, all heat transport takes place by conduction though water-saturated bentonite.

A few days after deposition, heat transport through the buffer is largely independent of the buffer heat capacity, and heat conduction in the buffer can be approximately described by the time-independent heat conduction equation:

$$\nabla(\lambda\nabla T) = 0 \qquad (2\text{-}1)$$

The most important parameter is thus the thermal conductivity, λ, of different parts of the system. The thermal conductivity of bentonite is primarily dependent on density, water saturation and mineral composition. The thermal conductivity of water-saturated MX-80 bentonite that has swelled out to its intended density, 2,000 kg/m^3, is about 1.2 W/(m·K) according to laboratory experiments.

The thermal conductivity of gaps filled with water is 0.60 W/(m·K), while that of gaps filled with gas, i.e. air and vapour, is about 0.03 W/(m·K). For the canister/bentonite gap the effective conductivity is 0.03–0.06 W/(m·K) taking into account also the contribution from the radiant heat transfer /Hökmark and Fälth 2003/.

Table 2-2 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can

Table 2-2. Process/variable table for the process Heat transport.

Variable	Does this variable influence the process?		Does the process influence this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Buffer geometry	Yes	Given as data in the thermal calculation	No	
Pore geometry	Yes	Given as data in the thermal calculation	No	Indirectly via temperature
Radiation intensity	No		No	
Temperature	No	Ignored	Yes	Result from the model (in time and space)
Water content	Yes	Given as data in the thermal calculation	Yes	Treated in 2.3.1
Gas content	No	Indirectly via water content	No	Indirectly via water content
Hydrovariables (pressure and flows)	No		No	Indirectly via temperature
Stress state	No		No	
Bentonite composition	Yes	Given as data in the thermal calculation	No	
Montmorillonite composition	No		No	
Pore water composition	No		No	
Structural and stray materials	May affect thermal conductivity	Neglected, since to be of any importance to the heat transport, there must be very significant amounts of non-buffer materials	No	

Buffer geometry: The resistance to heat transport in the buffer prior to its achieving water saturation is dependent on the distance between the canister and the deposition hole boundary, which entails changes in the temperature of the buffer if the dimensions of the canister hole or the location of the canister in the hole should be altered. After water saturation, however, the variations in geometry that could occur due to block fallout or a poorly centred canister have negligible effects. This is also true of effects of instantaneous or time-dependent deformations that can alter the geometry of the canister hole. Before water saturation, a poorly centred canister can be of importance for the distribution of gas-filled volumes and therefore for the temperature level and temperature distribution in the buffer.

Pore geometry: The geometry of the pore system will change slightly because of thermal expansion. The porosity, i.e. the volume fraction taken up by pores, influences the thermal conductivity. Equations (2-2) to (2-4) give approximate relations between porosity and conductivity.

Temperature: The influence of heat transport on the buffer temperature is obvious. If the heat transport is efficient, the temperature in the inner parts of the system will be lower than if there is a high thermal resistance. The temperature in the outer parts, however, is practically independent of the conditions in the interior of the deposition holes. Different models have been proposed for estimating the influence of the temperature on the thermal conductivity of bentonite /Knutsson 1983/. The overall effect is a small increase, which can for practical purposes be ignored.

Water content: The thermal conductivity of bentonite with a high montmorillonite content can be estimated with the aid of the Equations (2-2) to (2-4), which give the thermal conductivity as a function of the degree of saturation Sr and the porosity n, which, together with the mineral density, determine the density of the buffer /Knutsson 1983/.

$$\lambda = \lambda_0 + K_e (\lambda_1 - \lambda_0) \quad (2\text{-}2)$$

where

λ_0 = thermal conductivity at $S_r = 0$ (dryness)

λ_1 = thermal conductivity at $S_r = 100$ percent (water saturation)

$K_e = 1 + \log S_r$

λ_0 and λ_1 are determined according to Equations (2) and (3):

$$\lambda_0 = 0.034 \cdot n^{-2.1} \quad (2\text{-}3)$$

$$\lambda_1 = 0.56^n \cdot 2^{(1-n)} \quad (2\text{-}4)$$

Equation (2-1) gives values with an estimated accuracy of 20 percent and is valid for porosities larger than 0.15. A number of similar expressions relating thermal conductivity to saturation and porosity can be found in the literature /Börgesson et al. 1994/.

As long as there is heat transport and incomplete saturation, thermal gradients in the buffer may influence the state of saturation, such that the water content of the innermost parts of the buffer decreases temporarily due to moisture relocation to cooler regions further from the canister.

Gas content: The heat transport will not affect the gas content. The gas content in itself does not have any influence on the heat transport. If there is a gas phase, the effects of this will be just those of the incomplete saturation.

Hydro variables: Temperature variations will cause changes to the pore water pressure.

Stress state: Different models have been proposed for estimating the influence of increasing pressure on the conductivity of bentonite /Knutsson 1983/. They show a slight increase of the thermal conductivity, but the effect is not sufficiently verified to be credited /Börgesson et al. 1994/.

Bentonite composition: There is no dependence on the composition of the smectite. The presence of impurities may affect the thermal conductivity. To be of any importance, the impurity content must be high and the thermal properties of the impurities significantly different from those of the bentonite. High contents of quartz, for instance, will increase the conductivity.

Montmorillonite composition: Variability of the internal structure of the montmorillinite are unimportant to thermal conductivity.

Structural and stray materials: To be of any importance to the heat transport, there must be very significant amounts of non-buffer materials.

Boundary conditions

There are two boundary conditions:

- The heat flux from the local canister, determined by the power at the time of deposition and by the heat decay characteristics of the waste.
- The temperature at the walls of the deposition hole.

The distribution of the total heat output over the surface of the canister will depend on the way the initial canister-bentonite clearance develops. As long as the clearance, or part of the clearance, remains open, there will be some redirection of the heat flow towards regions with direct canister-bentonite contact, for instance at the canister base. In regions where the clearance is open, part of the flux will be due to heat radiation.

The rock wall temperature depends not only on the heat output from the local canister but also on the contribution from other canisters, on the rock thermal properties and on the repository layout.

Also at the outer interface, between buffer and deposition hole wall, gaps will occur during the saturation phase, and part of the heat transfer will be due to radiation.

After saturation, there will be direct thermal contact between canister and buffer and between buffer and rock, and all heat transfer will take place by pure conduction.

Model studies/experimental studies

Model studies. Predictions of the temperature evolution in the near field have been done analytically /Claesson and Probert 1996, Hökmark and Fälth 2003, Hedin 2004/ and numerically /Thunvik and Braester 1991, Hökmark 1996, Ageskog and Jansson 1999/.

These numerical studies have all generated consistent results. The temperature at the buffer/canister transition reaches a peak after about 10–30 years, depending on layout and rock thermal properties, while the rock wall peak temperature is reached after 30–50 years. If, for example the canister spacing is 6 m, the tunnel spacing 40 m, the canister power at the time of deposition 1,700 W and the rock thermal conductivity 2.8 W/(m·K), the maximum temperature increase at the wall of the deposition hole will be 50°C. The duration of the temperature pulse is a few thousand years. After 2,000 years the maximum excess temperature in the repository is 15–20°C, again depending on the repository layout and on the rock thermal properties. After 5,000 years, the maximum elevation in temperature from the initial ambient is about 10°C. After about 2,000 years, the thermal gradients in the near-field are almost zero.

/Hökmark and Fälth 2003/ and /Hedin 2004/ used results of different near-field thermal analyses as boundary conditions in numerical and analytical analyses of the heat transfer across the bentonitete buffer and across the different gaps. The results indicated that the effects of open canister-buffer gaps are more important than possible temporal and spatial variations of the heat transport properties within the buffer.

Experimental studies: /Börgesson et al. 1994/ measured the thermal conductivity of samples of compacted MX-80 bentonite by use of a heat pulse technique, Figure 2-1. The results verified the dependence on saturation and porosity suggested by the general expressions (Equations 2-1 through 2-3). The results match well with corresponding results obtained for similar materials, for instance the bentonite tested in the FEBEX experiment /Huertas et al. 2000/.

The Prototype Repository includes six full-scale deposition holes in two tunnel sections separated by a concrete plug /Goudarzi and Börgesson 2003/. There are two deposition holes in the outer section and four in the inner one. Inflow measurements performed prior to bentonite emplacement and start of the actual test showed that there are very significant differences between the individual holes. The supply of water to the two holes in the outer section is sufficiently low that after about 6 months of test operation the bentonite buffer is not close to saturation. The temperature drop across the still open canister/bentonite space in the dry holes is about 19°C. In at least one of the holes in the inner section, there are indications, e.g. no measurable temperature drop between canister and bentonite, that the annular space between canister and rock is almost saturated about two years after test start.

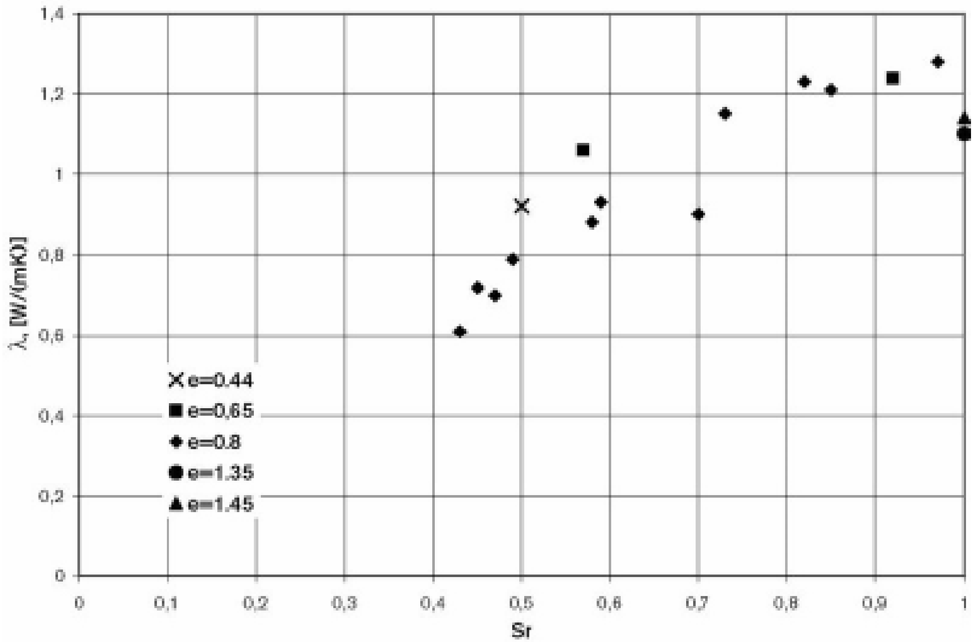


Figure 2-1. *Heat conductivity of laboratory–scale bentonite samples as function of saturation for a few values of the void ratio, e.*

The effective thermal conductivity λ_{eff} of the buffer in the annular space between canister and rock wall at canister mid-height can be estimated by use of the following expression:

$$\lambda_{eff} = \frac{q_c}{\Delta T} \cdot R_c \cdot \ln \frac{R_2}{R_1} \qquad (2\text{-}5)$$

Here ΔT is the temperature difference between two points at distances R1 and R2, respectively, from the heater axis. Rc is the canister radius. The canister surface heat flux qc at canister mid-height must be estimated from the total power and corrected to account for the non-uniform distribution of the heat output over the canister surface /Hökmark and Fälth 2003/. Applying the expression to the three holes described above using data reported by /Goudarzi and Börgesson 2003/ gives bentonite conductivity values ranging between 1.1 for the inner hole and 1.2 W/(m·K) for the two outer holes.

A similar estimate of the thermal conductivity of the bentonite in the canister retrieval test /Goudarzi et al. 2003/ gives a value of about 1.1 W/(m·K) 300 days–800 days after test start.

The TBT experiment in Äspö HRL is run under high thermal gradients and with maximum buffer temperatures well above 130°C /Goudarzi et al. 2005/. The buffer material is MX80 bentonite with the same properties (e.g. density and initial saturation) as the Prototype Repository bentonite blocks. The temperatures along a radial scan-line from the cylindrical, 0.6 m diameter, heater to the rock wall are monitored by use of numerous, densely positioned, thermocouples. Using Equation (2-5) above, the thermal conductivity along the scan-line is evaluated and used as an indicator of wetting/drying. The conductivity was found to be between 1.0 W/(m·K) and 1.1 W/(m·K) at the time of installation. It was between 1.1 W/(m·K) and 1.2 W/(m·K) after a little less than two years, except for in a 0.10–0.15 m wide zone around the heater. Close to the heater, the conductivity dropped to a minimum of about 0.6 W/(m·K) soon after installation and has increased to about 0.8 W/(m·K) after a little less than 2 years.

Natural analogues/observations in nature

Not applicable.

Time perspective

There are two relevant time perspectives: the water saturation perspective and the heat production perspective. The time it takes to achieve full water saturation is dependent on, inter alia, the pressure conditions in the groundwater in the near field. The process is estimated to take a number of years, see Section 2.3.1. After that, all heat transport takes place by conduction and under well-defined conditions with known thermal conductivities. Before then, heat transport can be influenced by the presence of gaps and joints.

After a few thousand years the heat production, and thereby the heat transport through the buffer, will have been reduced to a few percent of their original values.

Handling in the safety assessment SR-Can

The integrated thermal evolution of the fuel, cast iron insert, copper canister, buffer and rock will be modelled with the SR-Can near-field evolution model /Hedin 2004/.

An important purpose of the modelling is to evaluate the peak canister surface temperature that must not exceed 100°C, taking all relevant uncertainties into consideration. These include the possible presence of gaps between canister and buffer and between buffer and rock and data for describing heat conduction over these. Critical uncertain data for this evaluation will be given in the SR-Can data report. Another purpose is to obtain an estimate of the peak buffer temperature and of the buffer temperature as a function of time.

Time periods: The modelling will encompass at least 10,000 years, but the critical timescale is that period during which the peak canister temperature is reached, i.e. the first tens of years. For timescales beyond a few thousand years, it is important to determine if permafrost conditions could lead to freezing of the buffer, see further Section 2.2.2. This is done by a comparison of the rock thermal evolution during permafrost conditions to the buffer freezing temperature, taking the residual power of the canisters into account if relevant.

Boundary conditions: The treatment of heat transfer over the buffer boundaries is described in /Hedin 2004/ and /Hökmark and Fälth 2003/. As a special case, a poorly centred canister will be considered.

Handling of variables influencing the process: The process is coupled to the water saturation process (Section 2.3.1) which is difficult to model in detail, especially the evolution of gaps. Also, the water saturation process is highly dependent on the uncertain hydraulic conditions in the rock around the deposition hole. The peak canister temperature will therefore be determined under the assumption that no additional water is taken up by the buffer after deposition, i.e. a time independent, pessimistically chosen heat conductivity is used. Hereby, the influences of varying hydraulic conditions in the saturating buffer, including porosity variations, are pessimistically neglected. The thermal conductivity of the buffer will also be selected after taking into consideration the possible influence of impurities and presence of stray materials in the system. The gap between the canister and the buffer will conservatively be assumed to be open until the peak temperature has been reached.

Handling of variables influenced by the process: The temperature is explicitly calculated. The water content is handled in process 2.3.1.

The special cases of failed canister and of earthquakes: Canister failures and earthquakes of a magnitude that could affect the thermal evolution are not expected during the roughly 1,000 year time period in which the buffer temperature evolves significantly. The process is thus not handled for these cases. Should the assumptions regarding significant, early canister failures or earthquakes not be confirmed by the results of the safety assessment, the handling of the special cases will be reconsidered.

Uncertainties

Uncertainties in mechanistic understanding

Heat transfer from the hot canisters via the buffer to the near-field rock and backfill is in principle a simple process that can be described with reference to basic laws of physics. The character of the sub-processes that participate in the heat transport is also known and the theoretical modelling of their function is based on well-known physical principles.

Model simplification uncertainties for the above handling in SR-Can

Several modelling simplifications regarding the coupling to the hydraulic evolution are described under "Handling in the safety assessment" above. The conservative simplifications used in the models are justified since the prime purpose of the modelling is to obtain upper limits on canister and buffer temperatures. Sensitivity analyses will in some cases shed light on the effects of the simplifications.

Input data and data uncertainties for the above handling in SR-Can

Critical input data for the modelling of this process will be given in the SR-Can data report. Critical uncertain input data for use in determining the peak canister temperature include the heat power of the fuel, the thermal conductivity of the partly saturated buffer material and of the host rock. Also uncertainties of the emissivities of the inner buffer and in particular the outer copper surfaces are decisive in determining the peak canister temperature. Sensitivity calculations will be done to clairify the influence of various data uncertainties.

2.2.2 Freezing

Overview/general description

Frozen ground is defined as soil or rock having a temperature below 0°C. The definition is based solely on temperature and does not take into consideration whether water has been transferred into ice or not. When water undergoes phase change to ice, latent heat is released (334 J/g) and volume expansion takes place (approximately 9%). In a porous medium containing water in the pores, water will turn into ice if the temperature is low enough. Not all the water in the pores will freeze at a given temperature. At a given temperature equilibrium exists between water in ice phase and water still liquid. The amount of water in liquid phase is known as unfrozen water. The evidence establishing the existence of a continuous, unfrozen water phase that separates ice from the mineral matrix in porous media like soils is widely accepted /Anderson 1966, Miller 1963, Neresova and Tsytovich 1963, Williams 1964/. The amount of unfrozen water depends on various factors /Anderson and Tice 1972/ among which particle mineral composition, specific surface area of particles, temperature, presence of solutes and pressure are the most significant.

The primary factors governing phase composition can be written in order of importance as

$$w_u = \mathrm{f}(S, T, p, \pi) \qquad (2\text{-}6)$$

where S is specific surface area, T is temperature in degrees below 0°C, p is the mean total stress and π is the osmotic potential of the soil solution /Anderson and Tice 1972/. In addition to these four primary factors, a complete consideration would involve such secondary factors as the nature of the fine pore geometry of the grains, particle packing geometry and surface charge density.

The unfrozen water content increases with increasing specific surface area, temperature, stress level and solution concentration. For a given material the principal factor determining the unfrozen water content is the temperature. Stress level is less important, but a significant factor /Neresova and Tsytovich 1963, Anderson and Tice 1973/.

For a material with a given water content (w) the unfrozen water content (w_u) decreases with reduced temperature. The total water content, w is divided into two categories; the unfrozen water content w_u and the ice content w_i, (Equation 2-7). For temperatures close to 0°C all water remains unfrozen i.e. $w = w_u$. The temperature where ice starts to form is known as the "freezing point depression".

$$w = w_u + w_i \tag{2-7}$$

Numerous studies of the relationship between the unfrozen water content and temperature, for different types of soils, have been performed, see e.g. /Neresova and Tsytovich 1963, Anderson and Tice 1973, Andersland and Ladanyi 1994/.

It has been concluded /Anderson and Tice 1973/ that a convenient computation form of a general phase composition equation can be written as:

$$\ln w_u = 0.2618 + 0.5519 \ln S - 1.449\ S^{-0.264} \ln T \tag{2-8}$$

Equation 2-8 can be graphically presented as in Figure 2-2.

From Figure 2-2 it is clear that a material with a specific surface area of around 800 m^2/gram, the unfrozen water content at the temperature of –5°C is in the order of 35%. Some values of w_u as function of temperature and specific surface area are given in Table 2-3.

As long as the total water content is less than, or equal to, the unfrozen water content, no ice will be present in the system. As concluded by /Anderson and Tice 1972/, the freezing point depression vs. temperature can be regarded as equivalent to w_u vs. temperature. Table 2-3 and Equation 2-8 can therefore serve as a tool to determine the freezing point depression in the buffer material. This is valid as long as particle geometry can be regarded as an insignificant factor and ice is formed as Ice I (normal ice at pressure below 80 MPa). The assumptions are valid for the buffer material.

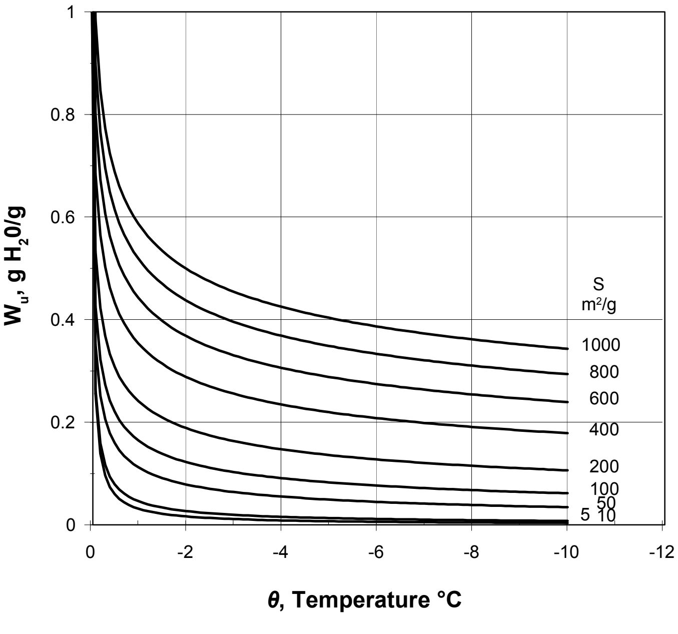


Figure 2-2. Unfrozen water content as function of temperature for various values of specific surface areas. After /Anderson and Tice 1972/.

Table 2-3. Unfrozen water content as function of temperature and specific surface area.

	Unfrozen water content, w_u (%)		
	600 m^2/g	800 m^2/g	1,000 m^2/g
Temp: – 1°C	44	52	59
Temp: – 2°C	37	44	50
Temp: – 5°C	29	35	40
Temp: – 10°C	24	29	34

All other factors influencing the unfrozen water content will increase w_u in relation to what is given in Table 2-3. Table 2-3 thus serves as a conservative estimate of the freezing point depression in the buffer material.

The average density at saturation of the buffer will be 2,000 kg/m^3 +/– 50 kg/m^3, which corresponds to a water content of 28% +/– 3%. With the specific surface area of 800 m^2/g, which is the estimated value for MX-80, all water is unfrozen down to below –10°C according to Table 2-3. However, there is an uncertainty in average density and in addition the buffer will not be homogeneous due to that the buffer is placed with empty and pellets filled slots and the friction in the material prevents complete homogenisation. According to (so far unpublished) measurements and modelling results the water ratio can vary between 25% and 32% in the buffer surrounding the canister. Considering also the uncertainty in initial average density the water ratio may thus vary between 22% and 35%. According to Table 2-3 all water will thus certainly be unfrozen until –5°C.

If ice is not present in the system, no increase in volume and no stress increase will take place and therefore questions related to ice lens formation will be of no relevance in the buffer. If the temperatures in the buffer at some time will be lower than 0°C, this will take place after complete water saturation of the buffer material. Since the water content at full saturation will be lower than 35% no ice formation will take place as long as the temperatures are above –5°C.

A high total stress on the buffer also helps in depressing the ice formation. The decrease is about 1°C per 13.5 MPa pressure, which thus means that the natural water pressure 5 MPa at the repository depth 500 m decreases the freezing point 0.4°C.

The effect of partly frozen pore water is an increased pressure from the buffer on the rock and canister due to the expansion of the water volume at ice and ice lens formation with additional pressure from growth of ice lenses. The effect of this is not well known and must be investigated if lower temperatures than –5°C are expected.

Table 2-4 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Boundary conditions

If the buffer freezes, the water in the backfill and rock will also be frozen. No redistribution of water will take place. The effect of freezing on the interaction with the backfill is not clear. There may be a fight for water.

Model studies/experimental studies

No studies on freezing of buffer materials have been done so far.

Table 2-4. Process/variable table for the process Freezing.

Variable	Does this variable influence the process?		Does the process influence this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Buffer geometry	If extended to regions with very low temperatures	Freezing of the buffer is excluded from SR-Can (see below)	Geometry could change through swelling towards the backfill	Freezing of the buffer is excluded from SR-Can (see below)
Pore geometry	Yes	“	Yes	“
Radiation intensity	No	“	No	“
Temperature	Yes	“	No	“
Water content	Via freezing point and transport capacity	“	If freezing takes place redistribution of water	“
Gas content	(A gas content would affect the process but the buffer will be completely saturated when freezing)	“	No	“
Hydrovariables (pressure and flows)	Freezing involves water transport	“	Yes	“
Stress state	Yes	“	Yes	“
Bentonite composition	The specific surface area	“	No	“
Montmorillonite composition	The specific surface area	“	No	“
Pore water composition	Influences the freezing point	“	No	“
Structural and stray materials	No	“	No	“

Natural analogues/observations in nature

This has not been done yet. However, knowledge can probably be achieved by studying permafrost areas.

Time perspective

When and if freezing occurs to repository depth the buffer will be completely water saturated. The water content will be lower than the freezing point depression and thus no ice will be formed in the buffer.

Handling in the safety assessment SR-Can

As the water content at full saturation will be lower than the unfrozen water content for temperatures higher than –5°C no ice will be formed and thus the process can be neglected.

Handling of variables influencing the process: A key issue is if freezing of the buffer can occur at repository level. A separate study of the conditions needed for a freezing process in the buffer and backfill at Forsmark and Laxemar have been performed within SR-Can. The temperature at repository level have been estimated within a Reference Glacial Cycle as well as within several colder scenarios more favourable for permafrost growth /Hartikainen 2004/ and /SKB 2006d/.

Handling of variables influenced by the process: The consequences of a frozen buffer/backfill will be evaluated within the SR-Can main report. If the temperature in the repository is below –5°C the resulting stress field and deformation will be estimated.

Handling of uncertainties in SR-Can

The long term effect of freezing of backfill materials has not been investigated in an organised way, which means that there are many uncertainties. A program for such investigations is underway.

2.3 Hydraulic processes

2.3.1 Water uptake and transport under unsaturated conditions

Overview/general description

Water transport in the buffer under unsaturated conditions is a complex process that is dependent on, inter alia, temperature, smectite content, degree of water saturation and water content in the different parts of the buffer. The most important driving force for water saturation under deep repository conditions is a negative capillary pressure in the pores of the buffer that leads to water uptake from the surrounding rock. The supply of water from the rock by water transport in fractures and in the rock matrix is also a decisive factor for the temporal evolution of the process.

Following is a detailed description of the process. The degree of detail is appropriate to indicate a general understanding, but is not necessary for the needs of the safety assessment to, for example, model the main features of the hydraulic evolution of the buffer.

The following hydraulic sub-processes can be distinguished:

- Transport of water in liquid phase, which is controlled and driven by
  A1) a pressure gradient in the water,
  A3) an osmotic gradient,
  A4) gravity (coupled to A1),
  A5) a density gradient (coupled to A1).
- Transport of water in vapour form, where transport is controlled and driven by
  B1) a pressure gradient in the water,
  B2) a temperature gradient,
  B3) an osmotic gradient,
  B4) gravity,
  B5) a density gradient.
- Phase transitions between water and vapour by:
  C1) evaporation,
  C2) condensation.
- Thermal expansion of
  D1) water,
  D2) air.
- Compression of
  E1) water,
  E2) air.
- Transport in water of
  F1) dissolved air.

These processes are coupled, and are in some cases different sides of the same process. They can be described and modelled in different ways. An important variable is the pore water pressure, which can be described according to Equation 2-9.

$$\psi \underset{.}{=} (u_a – u_w) + \pi \qquad (2\text{-}9)$$

where ψ is the free energy of the soil water (usually named total suction), u_w is the pore water pressure, u_a is the pore gas pressure and π is the osmotic suction. $(u_a – u_w)$ is called the matric suction.

The total suction can thus be described from a geotechnical viewpoint as the sum of the matrix suction, which can be said in simplified terms to stem from capillary effects, and the osmotic suction, which is dependent on differences in ionic concentration.

The driving force for water flow is usually considered to be the pore water pressure, which means that the matric suction and the pore gas pressure are important variables in the modelling of water flow in water unsaturated materials. The total suction is a function of the water content of the clay (called retention curve).

The understanding of the processes that drive water transport in unsaturated buffer and backfill materials and the knowledge of how the processes are influenced by different factors are not comprehensive. The following description (A1–A5, B1–B5, C1–C2, D1–D2, E1–E2 and F2) pertains chiefly to the models that are used for non-swelling soil materials /Fredlund and Rahardjo 1993/. It has not yet been fully clarified whether the approach is sufficiently all-inclusive to fully describe the processes in swelling clay minerals. However, the understanding is sufficiently good to carry out model calculations in the safety assessment.

A1. Transport of water in liquid phase, which is driven by a water pressure gradient, can be described by a refined version of Darcy's law. The parameters that control the process are the material's hydraulic conductivity K and the difference in pore water pressure u_w. Both of these can be described as functions of the void ratio e, the degree of saturation S_r, the ion concentration in the pore water i_c and the temperature T. The pore water pressure of unsaturated clays is also a function of the wetting history, i.e. whether the material undergoes wetting or drying, and the total average external stress.

A2. The primary driving force for the liquid-phase water flow is the pore water pressure gradient. The hydraulic conductivity varies strongly with the degree of saturation.

A3. Transport of water in liquid phase, which is driven by an ion concentration gradient, osmosis. Significant osmotic effects can arise at high salinities in the groundwater and in conjunction with salt enrichment in the buffer. The driving force should be visualised as a diffusion process driven by an osmotic gradient.

A4. Transport of water in liquid phase, which is driven by gravity. The influence of gravity is reflected in the hydraulic head and thus taken care of by process A1. Gravimetrically generated flow is probably negligible in both the buffer and backfill materials due to the low hydraulic conductivity, unless the liquid pressure originates from the water pressure in the rock.

A5. Transport of water in liquid phase, which is driven by a density gradient in the water. Differences in the density of the water can be caused by e.g. differences in temperature or salinity. Density-generated flow is probably negligible in buffer material, cf process A1.

B1. Transport of water in vapour phase, which is driven by a vapour pressure gradient. The vapour pressure u_v in the fraction of the pores that are air-filled or the relative humidity ($RH = u_v/u_{vo}$ where u_{vo} is the saturation pressure in the air) is in equilibrium with the total suction potential in the liquid phase. If RH is higher than the equilibrium relationship, water vapour condenses and increases the quantity of liquid, which in turn reduces the total suction until equilibrium arises. If the total suction differs in different parts of a soil, for example due to different water ratios, this leads to different vapour pressures, and transport of water vapour in the unfilled portion of the pores takes place with the vapour pressure difference as a driving force. At similar temperature and other circumstances water vapour is thus transported in the gradient of the relative humidity and (due to the direct correlation) in the gradient of total suction. However, this transport is parallel to process A1, which takes place in liquid phase. The relationship between these transport mechanisms has not been fully investigated.

B2. Transport of water in vapour phase, which is driven by a temperature gradient, appears to be the most important process for vapour transport. This process can also be regarded as a part of process B1. A temperature difference brings about a vapour pressure difference which transports vapour from a warmer part to a colder part. It can also be modelled as a diffusion process driven by a temperature difference /Philip and de Vries 1957/.

The vapour transport causes a water ratio difference and thereby a difference in suction potential, which in turn leads to a liquid-phase transport in the opposite direction. In a closed system, with a temperature gradient and constant mass of water, an equilibrium situation arises after a time where the vapour transport is equal to the liquid transport in all parts. A steady state arises with water ratio differences that reflect the temperature differences in the system.

B3. Transport of water in vapour phase, which is driven by an osmotic gradient. This is an indirect process since the vapour is driven by a difference in vapour pressure that can be settled by a difference in osmotic pressure.

B4 and B5.
Transport of water in vapour phase, which is driven by gravity or a density gradient. These processes are presumably insignificant in the buffer's pore system, but may be of great importance in gaps, particularly in the vertical gap between canister and bentonite.

C1 and C2.
Phase transitions via evaporation and condensation are constantly occurring in a temperature gradient where evaporation in the warmer part is accompanied by condensation in the colder part. Aside from the fact that it can lead to heat transport, it is only significant as evaporation if the buffer is not isolated from the atmosphere. It can occur if a very dry deposition hole is allowed to stand open towards the tunnel for a very long time or if the backfill is dry.

D1 and D2.
Thermal expansion of water in liquid and vapour phase can indirectly affect the flow by changing either the water pressure or the density (convection). Other consequences are dealt with under mechanical processes.

E1. Compression of water in liquid phase is of little importance for the liquid transport processes other than for a water-saturated system, where the size of the pressure build-up associated with a temperature increase is dependent on the compressibility of the water.

E2. Compression of air can be an important factor in the water saturation process (Boyle's law). If the air is trapped, it must be compressed and go into solution in the water in order for water saturation to be achieved. In highly compacted bentonite, the suction potential appears to be sufficiently high for this to occur and full water saturation is achieved without any external water pressure. Highly-compacted pure bentonite is thus able to achieve water saturation by itself. The backfill, however, has such low suction that a pressurized air volume will remain if the air cannot seep out. A large part will disappears when full water pressure has developed.

F1. Transport of dissolved air in water. When trapped air is compressed during the water saturation phase, a portion of the volume is dissolved in the water. This solubility (Henry's law) is approximately 2 percent at air temperature but decreases rapidly at increasing temperature. In order for additional air to be dissolved, the dissolved air must be transported away, which takes place by diffusion.

Influencing/Influenced variables

Influence of pore water composition on the wetting rate: High salinity in the groundwater that is absorbed from the near-field rock limits the swelling of the bentonite grains and initially leaves wider passages for penetration of water. The hydraulic conductivity increases with increasing salinity especially for low densities. An advantage is that saturation of the buffer can take place faster than if low-salinity water is absorbed.

The salinity of the groundwater influences the vapour pressure relation and thereby the water saturation process. For typical Swedish groundwater conditions, the effect in the buffer is small, but the influence of saline groundwater may be of decisive importance for water uptake in the backfill.

Influence of temperature on wetting rate: The viscosity of water is affected by the temperature, which means that the hydraulic conductivity increases with increasing temperature. This means that an increased overall temperature in the buffer increases the wetting rate.

Table 2-5 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Table 2-5. Process/variable table for the process Water uptake and transport under unsaturated conditions.

Variable	Does this variable influence the process?		Does the process influence this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Buffer geometry	Yes	Given as input data in saturation calculation	Influencing through the swelling of blocks	See 2.4.1
Pore geometry	Yes	Included in material data	Yes	State of saturation is calculated
Radiation intensity	No		No	
Temperature	Indirect through the water content and hydrovariables in a temperature gradient		Yes	Temperature as a function of time and space is calculated See also 2.2.1
Water content	Yes	Initial water content is given as input data in saturation calculation	Yes	State of saturation is calculated
Gas content	Yes	Initial gas content is given as input data in saturation calculation	Yes	State of saturation is calculated
Hydrovariables (pressure and flows)	Yes	Included variables in the saturation calculation	Yes	The pressure and suction is calculated
Stress state	Yes	Included variables in the saturation calculation	Yes	The pressure and suction is calculated
Bentonite composition	(Influenced through the retention curve)	Given as input data in saturation calculation	Unless via mineral conversion	Not relevant for saturation period
Montmorillonite composition	(Influenced through the retention curve)	Given as input data in saturation calculation	Unless via mineral conversion	Not relevant for saturation period
Pore water composition	Yes	Given as input data in saturation calculation	Yes	See 2.5.6
Structural and stray materials	Insignificant	Excluded	No	

Influence of water and gas content: The hydraulic conductivity is strongly affected by the degree of saturation. A commonly used relation between hydraulic conductivity and the degree of water saturation is provided in Equation 2-10.

$$K_p = S_r^{\delta} K \qquad (2\text{-}10)$$

where

K_p = hydraulic conductivity of partly saturated soil (m/s)

K = hydraulic conductivity of completely saturated soil (m/s)

δ = parameter ≈ 3 for MX-80 at buffer densities

The vapour diffusivity is also affected by the degree of saturation.

The pore water pressure in an unsaturated buffer is strongly affected by the water content (retention curve). For example: at w = 10% the pore water pressure is u ≈ –70 MPa while at w = 20% the pore water pressure is u ≈ –20 MPa. Under volume constrain the negative pore water pressure is reduced during water uptake and goes to 0 at complete water saturation.

Boundary conditions

Interaction with the rock: A key issue for the saturation process is the interaction between rock and buffer. If water is only conducted to the buffer in the water-bearing fractures and the rest of the water has to go through the rock matrix, water saturation can be both uneven and take a long time. If there is a permeable excavation-disturbed zone (EDZ) at the wall of the deposition hole, which distributes water from the fractures along the rock wall, the wetting will be faster and more even. However, tests performed to quantify this feature indicate that if diamond drilling is used for borehole excavation, there is only a small disturbance of the rock, which reaches a few cm into the rock but also that the disturbance is not of significant importance for the wetting. See e.g. /Autio et al. 2003/.

Interaction with the backfill: If the backfill is composed of a mixture of bentonite and crushed rock or similar, the suction is much higher in the buffer material than in the backfill. This means that if water inflow is very low that water may be transported from the backfill to the buffer and thus wet the buffer and dry the backfill. If the wetting of the backfill from the rock is faster than the wetting of the buffer, this water will also be redistributed to the buffer and thus help the wetting of the buffer. See e.g. /Börgesson et al. 2006/.

Model studies/experimental studies

A preliminary material model containing unsaturated water flow has been devised /Börgesson and Johannesson 1995/ and is being developed. The calculations are performed using the finite element method with the program ABAQUS. Certain general parts of the model are described in the manual /Hibbit et al./, while other parts are tailor-made for SKB. See e.g. /Börgesson and Johannesson 1995, Börgesson and Hernelind 1999, Börgesson et al. 2004a/. The model includes the processes A1, A4, A5, B2, D1 and E1, which are the most important ones for the buffer. It is a completely coupled thermo-hydro-mechanical model and thus also includes thermal and mechanical processes in the buffer. It does not, however, include the processes that handle air (except for B2), which can be important for the saturation process in the backfill.

The model has been both calibrated and partially verified by laboratory experiments. Models for unsaturated buffer have been evaluated within three international projects (DECOVALEX, CATSIUS CLAY and VALUCLAY). These projects included calculation examples and comparisons with measurement results for both laboratory experiments and field tests. See e.g. /Börgesson and Hernelind 1995, Alonso and Alcoverro 1997, Börgesson and Hernelind 1997, Börgesson et al. 2004a/.

In recent years another finite element program has been tested and used for thermal and hydraulic processes, namely Code_Bright /Cimne 2002/. This code was developed by UPC (Technical University of Catalonia, Barcelona). Most processes are similar to the processes in ABAQUS but there are some important differences. The main difference is that it can handle the gas phase and thus also model processes B1, B4, B5, D2, E2 and F1. It can also handle phase transitions (C1 and C2).

Several large-scale field tests have been installed with e.g. the purpose to study the wetting process of the buffer material in a repository.

The big field test BMT (Buffer Mass Test)) /Pusch et al. 1985a /was performed in the years 1981 to 1985 in Stripa, Sweden. In this test, highly-compacted bentonite and heaters were installed in six simulated, half-scale deposition holes. The tunnel above two of these holes was backfilled with sand-bentonite mixtures containing 10 and 20 percent bentonite. The tests were interrupted after a few years, whereupon buffer and backfill were excavated with detailed sampling and water ratio determination. The results showed that the wetting had gone to near water saturation in three of the holes, while the others had not increased their water content more than marginally. The water inflow in the three first-mentioned holes was greater than in the others. On the other hand, the gap towards the rock was left open in these three holes, while the gap in the three “dry” holes was filled with bentonite powder. There was no tendency towards uneven water uptake from the rock. The three wet holes with empty gaps had a high, uniform water ratio with a degree of saturation higher than about 80 percent. The three dry holes with powder-filled gaps were dry nearest the heater and wet nearest the rock, in a way that could be expected to result from the redistribution process that occurs in the presence of a temperature gradient.

In Äspö HRL several deposition hole tests with canister and buffer material are running but no test has so far been interrupted and excavated. These tests are the Canister Retrieval Test (CRT), the Prototype Repository and the Temperature Buffer Test (TBT) /SKB 2005c/. All tests simulate heating and wetting of the buffer. The CRT and TBT have artificial wetting of the buffer through filters covering all or parts of the rock surface, while the Prototype Repository has natural wetting from the rock. All six deposition holes in the Prototype Repository also have an upper boundary of backfill material that contributes to the wetting.

The wetting of the buffer in these tests have been modelled and, for the Prototype Repository, the influence of the rock structure and properties have been studied in detail /Börgesson and Hernelind 1999/. This study was originally done for the safety analysis but has also been used for the Prototype Repository. It is applicable for deposition holes in general. In the study the permeability of the rock matrix, the water supply from the backfill, the water pressure in the surrounding rock, the permeability of the disturbed zone around the deposition hole, the water retention properties of the rock, and the transmissivity of two fractures intersecting the deposition hole have been varied.

The results indicate that the wetting takes about 5 years if the water pressure in the rock is high and if the permeability of the rock is so high that the properties of the bentonite determine the wetting rate. However, it may take considerably more than 30 years if the rock is very tight and the water pressure in the rock is low. The calculations also show that the influence of the rock structure is rather large except for the influence of the transmissivity (T) of the fractures, which turned out to be insignificant for the values used in the calculations.

The results of the calculations show that the influence of most changes in rock properties and boundary conditions are rather large. There is a lack in knowledge of rock properties and interaction buffer/rock and a need for improved material models of the buffer.

Natural analogues/observations in nature

Wetting of bentonite in nature has not been studied and would probably not contribute to the knowledge necessary for water uptake assessment in a repository.

Time perspective

The above analyses show that the time to full water saturation of the buffer can vary a great deal, depending above all on the interaction with surrounding rock. For wet conditions in the host rock, saturation may be reached within 10 years. If there are no fractures and no supply of water from the backfill, all water has to go via the rock matrix, which may take 100 years in the granitic rock types occurring in Sweden.

The influence of the backfill material on the wetting of the buffer has recently been investigated in a number of calculations /Börgesson et al. 2006/. The main observations from these calculations are the following:

If wetting is achieved from the backfill (30/70) the time to full saturation of the buffer may be reduced with 50% at normal rock conditions.

In the extreme (and not applicable) case that no water at all is supplied by the rock (impervious rock) neither to the buffer nor the backfill all water must be taken from the existing water in the backfill. If 30/70 mixture with 12% water ratio (mass of water divided with the dry mass) is placed as backfill the water ratio will be reduced to about 11% and the degree of saturation in the buffer will be increased to about 98% in 1,000–2,000 years.

Another extreme case is that no water is supplied by the rock to the deposition hole but that a fracture zone intersecting the deposition tunnel results in rapid water saturation and a full water pressure of 5 MPa (in a repository located at 500 m depth) in the backfill. This scenario yields a time to saturation of 250–500 years.

Very long time until saturation is probably not a problem but the consequences have not been fully investigated. It can be divided into two cases:

1. No water can leave the deposition hole.
2. Water can leave the deposition hole and enter the backfill.

If water is supplied to the backfill or if the backfill has a naturally high RH (e.g. 30/70 with the water ratio 12%, which has an intial RH of 97%) the backfill and the swelling buffer in contact with the backfill will create a natural lid that does not allow any water to escape. Alternatively, if the backfill is composed of bentonite blocks with low RH, which are piled in the deposition tunnel, and if the deposition tunnel as well as the deposition hole are very dry, there is a possibilty that the hot environment around the canister in combination with slots between the blocks may dry the buffer and lead the moist air out into the backfill by mainly convection.

In case 1 (no water is allowed to leave the deposition hole) the consequence will only be an internal redistribution of water and attendant salt accumulation in the hot parts. This case is treated in Section 4.7.

Case 2 combined with a slow water inflow into the lower part of the buffer may lead to a salt accomulation in the buffer around the canister that is far stronger than if only internal redistribution takes place.

Handling in the safety assessment SR-Can

The initial THM evolution covering the saturation phase of the buffer will be modelled for a number of hydraulic boundary conditions in SR-Can since the supply of water at the outer buffer boundary is decisive for the wetting rate. Calculations will be made both with the old THM-model used for SR-Can /Börgesson and Hernelind 1999/ and updated models, e.g. with Code Bright. The purpose of these calculations is to study the sensitivity of rock and backfill properties to the wetting time of the backfill and the indirect influence on the wetting of the buffer. The outcome will be increased knowledge how much different processes and propertiesz influence the saturation time.

The near-field evolution model /Hedin 2004/ as well as finite element models /Börgesson et al. 2006/ have be used to study the swelling of the buffer and the compaction of the backfill at the end of the saturation phase for different assumptions regarding critical input data like friction, swelling pressure and groundwater salinity. These studies have been done since one of the critical results of the swelling at the end of the saturation phase is the redistribution of buffer mass leading to a reduction of buffer density at the top of the deposition hole.

Timescales: The THM modelling will encompass the wetting period for the backfill and buffer. The detailed timescale will consequently be determined by the hydraulic conditions in the bedrock, which control the wetting. Typical timescales range from less than ten to more than a hundred years.

Boundary conditions: The THM modelling will be performed for a number of different hydraulic conditions in the bedrock.

Handling of variables influencing this process: The process is coupled to a number of other processes in the THM model. The modelling will be done for a realistic thermal gradient over the buffer and include thermal expansion. All variable influences in Table 2-5 above will be included in the modelling except effects of varying pore water composition. It is recognized that the salinity of the pore water could influence the final swelling of the buffer. This is however included in the near-field evolution model where the salinity effect on swelling is implemented according to Section 2.5.8 (osmosis).

Handling of variables influenced by the process: The buffer saturation as a function of time as well as the swelling of the buffer at the end of the saturation process (considering friction between buffer and the wall of the deposition hole), the associated compaction of the backfill and possible movements of the canister in the deposition hole as a consequence of these phenomena will be caculated.

The special cases of failed canister and of earthquakes: Canister failures and earthquakes of a magnitude that could affect the wetting process are not expected during the time period in which the buffer saturates. The process is thus not handled for these cases. Should the assumptions regarding significant, early canister failures or earthquakes not be confirmed by the results of the safety assessment, the handling of the special cases will be reconsidered.

Uncertainties

The knowledge of the hydraulic behaviour of unsaturated buffer material is gained from investigations done on MX-80 while almost no tests have been performed on the other buffer candidate (Deponit CA-N bentonite). At the density considered for the buffer material the behaviour is similar but this needs to be confirmed.

Uncertainties in mechanistic understanding

The understanding of the process is deemed sufficient for the needs of the safety assessment. Some hydraulic parameters and processes in the buffer are uncertain e.g. the suction close to water saturation and the influence of the swelling pressure (currently being studied), the influence of entrapped air and the magnitude of vapour flux and the influence of gaps, which imply very inhomogeneous initial conditions. Although detailed knowledge of these processes might not be needed for the safety assessment they will be studied in order to gain further confidence in the wetting modelling.

Model simplification uncertainties for the above handling in SR-Can

The water uptake modelling done so far has assumed that the bentonite blocks and the slots (filled or unfilled) are homogeneous so that the buffer has the same density everywhere from start. This simplification is not correct but the effect of the error is likely to be smaller than that of the uncertainty of the rock properties.

The detailed description of the wetting process is complicated, but it can be modelled with sufficient accuracy for the needs of the safety assessment for which it is not important to know all the details of the process. It is however important to show that full water saturation is eventually reached in order to provide a reliable description of the long-term evolution following saturation and to determine the distribution of buffer and backfill mass at the end of the saturation phase. It is further important to assess the possible chemical alterations of the buffer during the saturation process. Such alterations are however not expected to influence the saturation process and need hence not be considered for this process.

Input data and data uncertainties for the above handling in SR-Can

The greatest uncertainty/variability concerns the hydraulic conditions in the near-field rock and the hydraulic interaction between the rock and the buffer. This will be addressed by analysing a number of cases with differing assumptions regarding these properties.

2.3.2 Water transport under saturated conditions

Overview/general description

Water transport in saturated buffer is a complex interplay between several sub-processes on a microscopic scale. On a macroscopic level, the result is that the permeability of a saturated buffer is very low, and this is also the essential result for the safety assessment.

Water flow in saturated buffer is a special case of unsaturated flow. The processes involved are the same as for unsaturated conditions, but can vary widely in importance compared with unsaturated conditions.

The most important mechanism under saturated conditions is transport of water in liquid phase, which is driven by a water pressure gradient. This transport process can be described by Darcy's law. Any deviations from Darcy's law, which can occur at low gradients, are favourable in that they lead to a reduced through flow rate. See e.g. /Dixon et al. 1999/ and /Hansbo 1960/. The hydraulic conductivity K is a function of the composition of the buffer, the void ratio, e, the ion concentration in the pore water, i_c, and the temperature, T.

The hydraulic conductivity of the reference buffer (MX-80 and Deponit CA-N) to low-salinity water after complete saturation is approximately 10^{-13} m/s at the density 2,000 kg/m^3 at water saturation (see below).

An approximate condition for transport by flow to be more important than diffusive transport is given by: $D_e/\Delta L < Ki$, where D_e = the effective diffusivity, ΔL = the transport length (one-dimensional), K = the hydraulic conductivity and i = the hydraulic gradient. For the stage after restoration of the hydraulic situation in the repository, i can be set equal to 10^{-2} and, for anions $D_e = 10^{-12}$ m^2/s, which for the buffer thickness $\Delta L = 0.35$ m requires that K exceeds $3 \cdot 10^{-10}$. This value of K is at least two orders of magnitude higher than the real conductivity of the buffer. The margin for cations, which have a lower diffusivity, is considerably greater. The conclusion can therefore be made that the only important transport mechanism for both water and dissolved species through the buffer is diffusion. Diffusive transport is dealt with in Section 2.5.3.

The requirement to have a hydraulic conductivity that is so low that advection (flow) can be neglected has led to a demand of the hydraulic conductivity of the buffer of

$K < 10^{-12}$ m/s,

which is about 2 orders of magnitude lower than theoretically required for the mass transport process to be diffusion-dominated. Since this demand can only be fulfilled if all initially-present slots or gaps are healed and there is a perfect contact between the buffer and the rock. A requirement for a minimum swelling pressure σ_s in the system also exists and is:

$\sigma_s > 1$ MPa

This value is chosen since the hydraulic conductivity is clearly lower than 10^{-12} m/s at that swelling pressure. 1 MPa is also high enough to efficiently fill irregularities on the rock surface in a deposition hole.

Influencing/influenced variables

Table 2-6 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.
Influence of density, temperature and salinity:

The hydraulic conductivity is primarily dependent on the geometry and composition of the buffer, the density (expressed in Table 1 as water content), the ion concentration in the pore water and the temperature.

In the buffer, $K = 5 \cdot 10^{-14}–5 \cdot 10^{-13}$ m/s at the densities in question both for MX-80 and Deponit CA-N bentonite. The dependency on density is rather strong. Figure 2-2 and Figure 2-3 show the hydraulic conductivity of MX-80 and Deponit CA-N bentonites measured at different densities and with different ion concentration in the saturating solutions. Blue markers indicate pure water conditions, and these results consequently show the effect of the originally clay mineralogy including original cations. The other markers show the results with chloride solutions of the dominant cation in the two clays, respectively. Additional tests show that ion exchange of MX-80 clay to a calcium state leads to hydraulic conductivity similar to those in the original Deponit CaN material, and ion exchange of Deponit CaN clay to sodium sate leads to hydraulic conductivities similar to those in the original Mx-80 clay.water.

Transformations to other minerals with reduced montmorillonite content as a result generally lead to a higher hydraulic conductivity. The temperature influences the conductivity by changing the viscosity of the water, whereby a temperature increase from 20°C to 90°C entails an approximate increase in conductivity by a factor of 3. The influence of salinity on the hydraulic conductivity is at buffer densities not very strong. Investigations are ongoing as shown in Figure 2-3 and. Figure 2-4.

Boundary conditions

The outer boundary conditions are determined by the hydraulic properties of the rock surrounding the deposition hole, in particular the properties of possible fractures intersecting the deposition hole and of the excavation damaged zones that may exist in the peripheries of both deposition holes and deposition tunnel floor.

Model studies/experimental studies

Flow in water-saturated buffer has been studied on a laboratory scale in the form of permeability tests and swelling/compression tests in oedometers /Börgesson et al. 1995, Karnland et al. 2006/.

Natural analogues/observations in nature

No studies of water flow in natural buffer like formations have been done on several reasons, the main ones being that the measured values are very low compared to the requirements and that changes in hydraulic conductivity with time will be a consequence of chemical alterations that are treated in other chapters. However, such studies should be considered because they may yield valuable information about long term behaviour.

Table 2-6. Process/variable table for the process Water transport under saturated conditions.

Variable	Does this variable influence the process?		Does the process influence this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Buffer geometry	Yes	Given as input data. The effect of the geometry, meaning how the buffer expands into other volumes (the backfill) is described in Section 2.4.1.	No	
Pore geometry	Yes	Determines the hydraulic conductivity (see text) The pore geometry can be affected by a mineral transformation or a change in porewater composition. The effects are discussed in Sections 2.5.9 and 2.5.8	No	
Radiation intensity	No		No	
Temperature	Yes	The increase of hydraulic conductivity as function of temperature is about a factor 3 between 20°C and 90°C. This will be neglected in SR-Can because the thermal pulse will be over when any significant amount of radionuclides may have entered the buffer	No	
Water content	Influenced via density	Determines the hydraulic conductivity (see text)	No	
Gas content	(Dissolved gases)	Excluded, would reduce conductivity	No	
Hydrovariables (pressure and flows)	Yes	The hydraulic gradient determines whether advection can occur	Yes	Diffusion only for intact buffer. If the hydraulic conductivity present once the process is taken into accout is below 10^{-12} m/s, and the swelling pressure above 1 MPa, advection will be neglected. If the hydraulic conductivity and/or the swelling pressure do not meet the assigned function indicators, it has to be evaluated as if advection could be of importance to the system.
Stress state	No		No	
Bentonite composition	Yes	Determines the hydraulic conductivity (see text)	No	
Montmorillonite composition	Yes	Determines the hydraulic conductivity (see text)	No	
Pore water composition	Yes	Determines the hydraulic conductivity (see text)	Yes	Replacement of porewater is discussed in 2.5.6
Structural and stray materials	(Insignificant)		No	

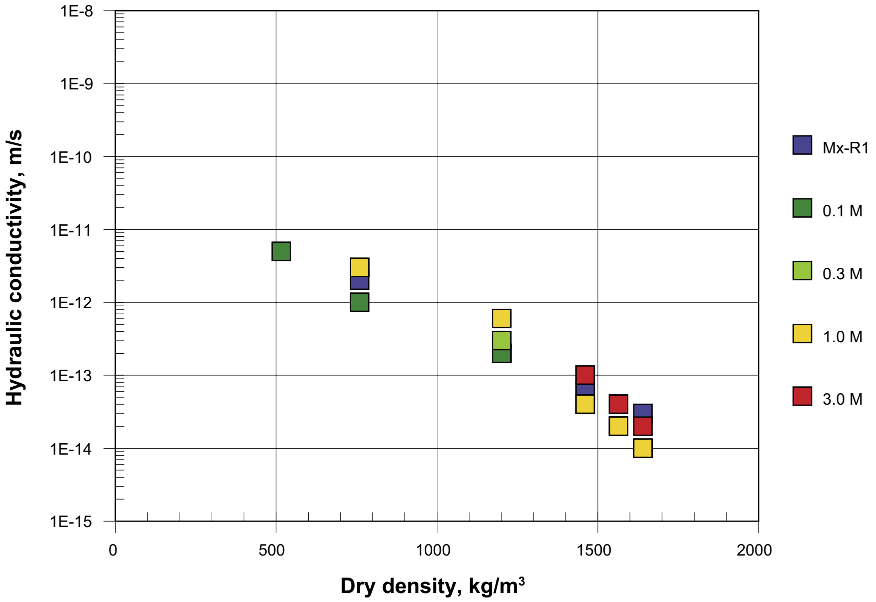


Figure 2-3. *Hydraulic conductivity of MX-80 bentonite measured at different densities and molar concentration of NaCl in the saturating solution.*

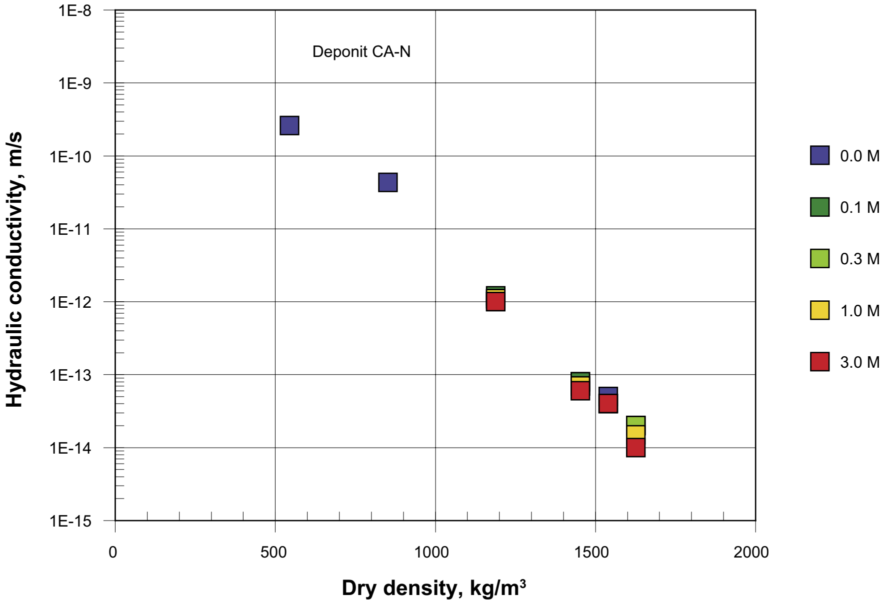


Figure 2-4. *Hydraulic conductivity of Deponit CaN bentonite measured at different densities and molar concentration of* $CaCl_2$ *in the saturating solution.*

Time perspective

The hydraulic gradient that exists after water saturation and pore pressure equilibrium have been reached around a repository is expected to be low. A simple estimate can be made of the time required for all the water in the buffer to be exchanged. If the gradient is set to 0.01, the hydraulic conductivity K to 10^{-13} m/s and the cross-sectional area to 10 m^2, according to Darcy's law it takes 15 million years for the approximately 5 m^3 of water present in the buffer to be exchanged. Transportation and exchange of ions via advection is thus a slow process compared to ion diffusion (see Sections 2.5.2 and 2.5.3).

Handling in the safety assessment SR-Can

The primary handling of this process will be to consider how the hydraulic conductivity could vary for the evolving conditions in the buffer throughout the assessment period and to compare the values with the function indicators.

Time periods: After saturation and throughout the assessment period.

Handling of variables influencing this process: The evolution of buffer density, temperature and ionic composition will be studied and the hydraulic conductivity and the swelling pressure will be evaluated for the changing conditions caused by the chemical evolution and alterations of density:

- The effect of the geometry, meaning how the buffer expands into other volumes (the backfill) is described in Section 2.4.1.
- The pore geometry can be affected by a mineral transformation or a change in porewater composition. The effects are discussed in Sections 2.5.9 and 2.5.8
- The increase of hydraulic conductivity as function of temperature is about a factor 3 between 20°C and 90°C. This will be neglected in SR-Can because the thermal pulse will be over when any significant amount of radionuclides may have entered the buffer.
- The hydrovariables will be used to calculate the flow in the buffer
- The amount and composition of the swelling component in the bentonite will be evaluated according to Section 2.5.9.
- The effect of a change in groundwater/porewater will be evaluated according to Section 2.5.8.

A combiniation of several factors will also be discussed.

The conductivity will be evaluated by application of the empirical relationships described above.

Handling of variables influenced by the process: If the hydraulic conductivity present once the process is taken into accout is below 10^{-12} m/s, and the swelling pressure above 1 MPa, advection will be neglected.

If the hydraulic conductivity and/or the swelling pressure do not meet the assigned function indicators, it has to be evaluated as if advection could be of importance to the system. In this situation, advective transport will be included in the calculations for corrosion and radionuclide transport.

Boundary conditions: The hydraulic gradient for altered conditions during permafrost and glaciation will be estimated.

The special cases of failed canister and of earthquakes: These are handled via possible mass redistributions, see Section 2.4.1. Pressure transients may cause liquefaction under rather extreme conditions. Liquefaction is treated in Section 2.4.2, which concludes that the possible pressure increase is too low to cause liquefaction but also that the theories behind that conclusion needs to be further verified.

Uncertainties

So far very few tests have been performed on Deponit CA-N bentonite but those results available indicate that the properties of this material are very similar to the properties of MX-80 at the densities considered for the buffer material (see Figure 2-4).

Uncertainties in mechanistic understanding

An uncertainty exists as to whether Darcy's law applies at the low hydraulic gradients that are expected to arise, since all laboratory tests are done at very high gradients. All measured deviations show, however, that the flow is lower than is expected by application of Darcy's law to results obtained at high hydraulic gradient (see e.g. /Dixon et al. 1999, Hansbo 1960/).

Another uncertainty is the effect of transformations, which for some cases are expected to give higher hydraulic conductivity. The effects of very high salinities are also inadequately understood.

Model simplification uncertainties for the above handling in SR-Can

The model used is empirical, connecting hydraulic conductivity to temperature, density and ionic strength of the pore water. The uncertainties in this description are primarily given by the uncertainties of the empirical relationships on which the model is based. The primary aim is to establish that the transport through diffusion is considerably more important than advective transport, meaning that the exact value of the hydraulic conductivity is a secondary concern.

Input data and data uncertainties for the above handling in SR-Can

Input data for the study of hydraulic conductivity are primarily the empirical relationships between hydraulic conductivity and density, temperature and pore water composition described above. The primary aim is to establish that the transport through diffusion is considerably more important than advective transport, meaning that the exact value of the hydraulic conductivity is a secondary concern.

2.3.3 Gas transport/dissolution

Overview/general description

Transport of gas in the buffer can occur in two phases of the repository's evolution:

- When the repository is sealed, air will be trapped in the buffer. As the buffer becomes saturated with water, the air must escape.
- If a canister should be defective such that water could penetrate through the copper shell, the cast iron insert is expected to corrode, resulting in hydrogen gas formation. If more hydrogen is produced than can be dissolved in the water in the canister, a gas phase will form.

Gas which is trapped in or by the buffer can escape by two principal mechanisms:

- If the production rate is low or the gas quantity small, the gas can be dissolved in the pore water and be removed by diffusion.
- If the production rate is higher or the gas quantity is larger than can be removed via dissolution and diffusive processes, a gas phase will form, the pressure will rise, and a flow path is expected to be formed through the buffer at a critical pressure.

Water saturation phase: Gas flux in conjunction with wetting of the buffer is described in Section 2.3.1. Under these conditions, all gas originally present in the buffer is expected to be dissolved in the buffer's pore water and transported by diffusion.

Gas transport from failed canister before saturation: Before the buffer is saturated, water is only expected to be able to get into an assumed damaged canister via vapour-phase diffusion. Hydrogen production from corrosion will therefore be limited and the gas that is formed is expected to be able to leave the buffer via diffusive transport. The gas transport resistance in an unsaturated buffer is also considerably lower than in a saturated one (Canister damages at this early stage are very unlikely and so this process is considered to be very unlikely).

Gas from defective canister after saturation:

Diffusion: Hydrogen gas formed by corrosion of the cast iron insert can dissolve in the pore water and migrate from the canister by diffusion. The maximum transport capacity for different conditions has been estimated by /Wikramaratna et al. 1993/.

The results of the calculations show that the diffusive transport capacity is considerably lower than the hydrogen gas production from corrosion, if it is assumed that the entire surface of the cast iron insert is accessible for corrosion and the water supply does not limit corrosion. Under such conditions it is probable that a gas phase will be formed inside the canister and that the gas must escape by gas-phase flow.

Gas flow: The following picture of the subsequent course of events is an interpretation of the results of theoretical and experimental studies: At a critical pressure (entry pressure), the buffer is expected to allow the gas to pass through. When the pressure reaches this value, a transport pathway is formed through the buffer and gas is released. If gas production is maintained, the pressure will fall to a steady-state pressure. When the production ceases the pressure falls, and if the gas production is low enough, the transport pathway is expected to close. This takes place at a so-called "shut-in pressure", which is belived to be dependent on the swelling pressure. At pressures lower than the shut-in pressure, gas migrates solely by diffusion.

Gas entry, breakthrough, peak and steady-state gas pressures in the buffer are dependent on the properties of the buffer. The most important parameters seem to be the swelling pressure, the mechanical properties of the buffer and the stress situation.

Based on the experimental interpretation by /Harrington and Horseman 2003/, at the peak pressure a fracture will open and the peak pressure could be expressed as:

p_g (peak) $= T + 2\sigma_{eff} + p_w$

according to the 'classic theory' of hydrofracture in rock /Haimson and Fairhurst 1967/. Applying this process to the clay buffer, T is the tensile strength of the clay, σ_{eff} is the isotropic effective stress outside the region of stress concentration and p_w is the porewater pressure in the clay.

In the post-peak region, the bentonite will have lost its tensile strength normal to the plane of the fracture. The gas pressure is now equal to the total stress, σ. On this basis, the gas pressure at any point on the post-peak transient can be written as:

p_g (post-peak) $= \sigma = \sigma_{eff} + p_w$

At the (near) steady-state condition, the gas permeability of the fracture network must remain more or less constant with time, with no tendency for crack dilation or closure. Conceptually, the fracture must be propped open at any point along its length by the local gas pressure.

When gas production ceases, gas pressure drops and then gradually falls away along a very protracted pressure transient. The gas pressure and total stress are approximately equal at all points along the transient.

As gas pressure decreases, individual flow pathways should collapse leading to declining overall gas permeability. The gas pressure cannot fall below the sum of the capillary pressure, p_c, and the externally-applied water pressure (backpressure), p_{we}, or:

p_g (shut-in) $= p_c + p_{we}$

where p_c is the capillary pressure, which is equal to the swelling pressure. This provides a lower bound value for the gas pressure at shut-in.

The energy that drives the gas transport comes from compression of the gas inside the canister and is proportional to the available gas volume. If it is assumed that the volume is a cubic metre and the gas pressure drops from 12 to 9 MPa, 30 MJ will be released when the transport pathway is formed. In a system with confined clay (deposition holes), the gas will presumably be released in a controlled fashion, i.e. it will not entrain the buffer material along with it, but experiments under open conditions, i.e. without surrounding counter-pressure, show that gas breakthrough can be a violent process /Donohew et al. 1998/.

Available experimental results show that gas can migrate through a highly-compacted buffer without jeopardizing the continued function of the engineered barriers. However, no experiment has been conducted with a gas volume equivalent to the volume in the canister cavity (approximately 1 m^3), and it is therefore not completely clear what effect the release of large quantities of gas will have on the performance of the repository.

Table 2-7 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Table 2-7. Process/variable table for the process Gas transport/dissolution.

Variable	Does this variable influence the process?		Does the process influence this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Buffer geometry	Yes	The importance of the buffer volume on gas transport is unknown	It is important to demonstrate that the gas does NOT influence the buffer geometry	
Pore geometry	Yes	Is assumed to determine break through pressure	Fracturing from gas transport	No effect on water transport is assumed
Radiation intensity	No		No	
Temperature	Yes	Gas pressure is temperature dependent. This will be neglected since gas transport will take place after the thermal period	No	
Water content	Yes	The gas permeability of the bentonite is strongly dependent on the water content. This will be neglected since gas transport will take place after the saturation phase	No	
Gas content	Yes	See water content	Yes	The de-saturation effect is assumed to be small Diffusive transport of hydrogen is considered
Hydrovariables (pressure and flows)	Yes	Gas pressure and hydrostatic determines whether gas can be transported through the buffer	Yes	The gas pressure is a component in the total near field pressure
Stress state	Yes	The swelling assumed to determine break through pressure	Yes	The gas pressure is a component in the total near field pressure
Bentonite composition	Indirect influence through stress state		No	
Montmorillonite composition	Indirect influence through stress state		No	
Pore water composition	Indirect influence through stress state		No	
Structural and stray materials	No		No	

The gas transport resistance in an unsaturated buffer is considerably lower than in a saturated one. Tests on unsaturated Avonlea bentonite have shown breakthrough pressure to be negligible below a degree of saturation of around 80 to 90% /Hume 1999/. This range marks the saturation at which there are no continuous gas channels through the clay. In Kunigel VI bentonite, the critical saturation for interconnected gas voids was found to be 72% /Tanai et al. 1997/.

Boundary conditions

The essential boundary conditions for this process are the geometries of the conducting features at the buffer interfaces to canister and rock around the deposition hole and the pressure and volume of gas trapped inside the inner interface. The geometric aspects of these boundaries include the nature of the opening in a defective canister, fractures intersecting the deposition hole and excavation damaged zones around deposition hole and in the floor of the deposition tunnel.

When the gas has reached the excavation-disturbed zone (EDZ) in the near-field rock, the pressure required to get it to migrate further is much lower than in the buffer. It must exceed the sum of the water pressure and the capillary tensions in the fine fractures in the EDZ or in channels in fractures that intersect the deposition holes, which together gives a pressure of 5–10 MPa.

Model studies/experimental studies

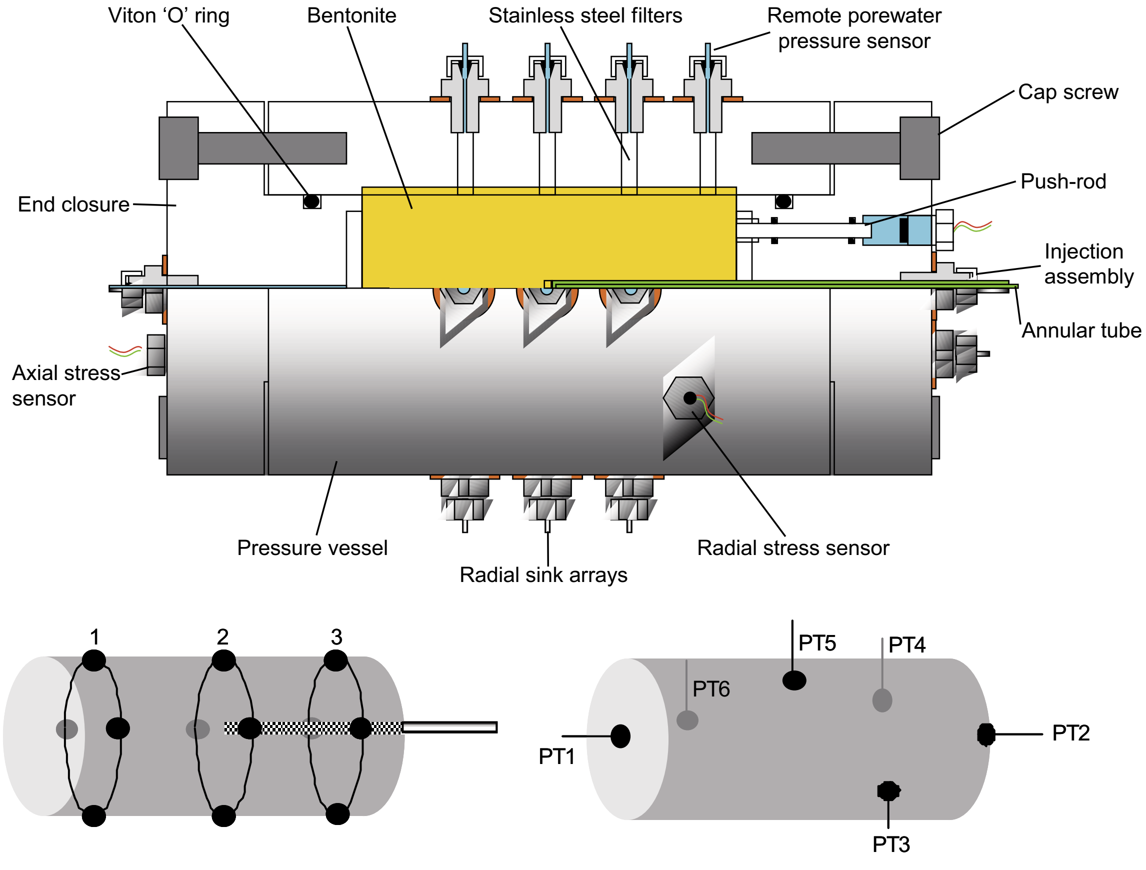
Gas dissolution: No specific studies have been conducted for the purpose of studying how gas dissolves in the pore water in the bentonite. However, experience from water saturation tests shows that highly-compacted bentonite normally achieves complete water-saturation and that no trapped gas remains. The mechanistic interpretation is that the swelling pressure of the bentonite compresses trapped gas, which is dissolved in the pore water and this gas is ultimately transported away by diffusion.

Gas transport: A number of gas migration experiments in compacted clays, with different materials, geometries and boundary conditions, have been performed over the last 20 years. Several of these are summarized in /Harrington and Horseman 2003/.

/Harrington and Horseman 2003/ presents the most recent gas migration experiments within the SKB programme. In the test geometry, the specimen was volumetrically constrained, preventing dilation of the clay in any direction. Figure 2-5 shows the actual test set up.All bentonite specimens were fully hydrated before gas testing by backpressuring using de-aired and distilled water. This procedure gave initial degrees of saturation that were demonstrably close to 100%. Figure 2-6 shows the gas injection history from one of the tests.

Gas testing began by pumping gas into the upstream system at a rate of 375 $\mu l \cdot hr^{-1}$. All filters, other than the central source filter and the radial sink filters, were closed off during gas testing. A very small amount of flow was observed at a gas pressure of 13.8 MPa, accompanied by a slight increase in axial and radial total stress. Gas pressure continued to rise until major gas entry occurred at a gas pressure of 18.9 MPa. Injection gas pressure momentarily dropped to 18.7 MPa and there was a sharp rise in axial total stress from 1.6 MPa to 18.3 MPa. Gas pressure then continued to rise to a peak value of 19.4 MPa, at which point large quantities of gas began to flow to the sink array [1] (see Figure 2-5). It would appear that the first gas pathway did not intersect a sink and a short period of growth was required in order to obtain gas breakthrough.

It should be noted that the measured peak pressures in these constant volume test are substantially higher than the ones measured in the earlier constant stress experiments.



Sink configuration **Stress sensor locations**

Figure 2-5. *Cut-away diagram of the constant volume and radial flow (CVRF) gas migration apparatus. [1], [2] and [3] indicates the radial sink arrays. Sensors are as follows: [PT1] – axial total stress on the backpressure end-closure, [PT2] – axial total stress on the injection end-closure, [PT3] – radial total stress close to the injection end-closure, [PT4] – porewater pressure close to the injection end-closure, [PT5] – radial total stress at the mid-plane, and [PT6] – radial total stress close to the backpressure end-closure.*

There is strong evidence that gas flows through a network of pressure-induced pathways. Very little, if any, displacement of water occurs during gas movement. The crack-like pathways are propped open by the elevated gas pressure. When gas pressure falls, individual pathways can snap shut leading to a reduction in overall gas permeability. What is absolutely clear from these gas injection experiments is that it is possible to pass up to 60 litres (STP) of helium through specimens of buffer clay (at gas pressures of over 8.0 MP for times in excess of 5 months) without any measurable desaturation occurring. This strongly reinforces the observations made by others on the lack of desaturation occurring during gas flow through fully hydrated bentonite.

There is no evidence from these tests that the development of pressure-induced gas pathways in any way compromises the sealing capacity of the bentonite barrier. Gas pathways are ephemeral features of the buffer that tend to close up when gas pressure falls. Breaks in slope of monitored pressure transients can be interpreted as discrete pathway 'sealing' events that coincide with decreases in the rate of discharge of gas to the sinks. More importantly, a history of gas movement through the buffer has been shown to have no detectable effect on permeability to water.

A consortium of radioactive waste disposal agencies, the GAMBIT Club, has been supporting efforts to develop an appropriate model of gas migration through bentonite, with the objectives that the model (a) should adequately represent the principal features observed in experiments of gas migration through compacted bentonite, (b) can be used to analyse and interpret

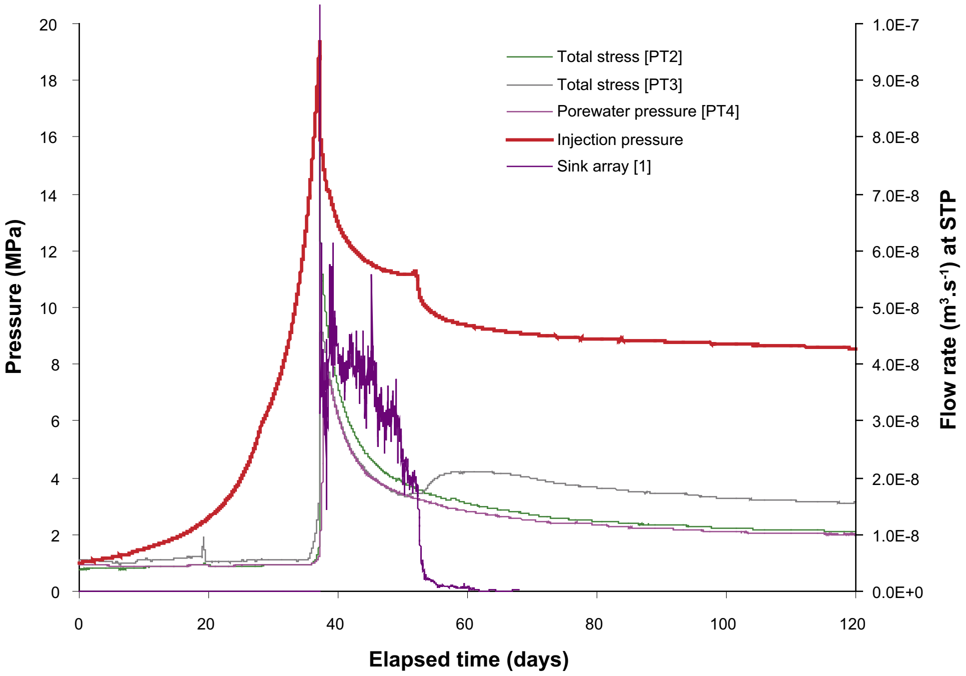


Figure 2-6. *Gas injection pressure versus time for the first breakthrough and shut-in stages of test Mx80-8, showing axial and radial total stress, porewater pressure and flow rate from sink array [1] (Figure 2-5). Flows to sink arrays [2] and [3] were too small to be distinguished when plotted on this scale. Mass balance considerations show that the flow from sink array [1] is predominantly gas.*

experimental results, and (c) will provide the basis of a model that can be used to assess pressure build up and escape of hydrogen gas through bentonite around waste canisters in a repository /Rodwell et al. 2003/. From that study a number of conclusions can be drawn:
A model in which gas migration in highly compacted bentonite occurs by fissure propagation is able to account qualitatively for the behaviour seen, although heuristic arguments are required to explain the dependence of the gas permeability on gas pressure after breakthrough, and the model is limited in the range of phenomena it portrays.

a) In order to explain the observed experimental results based on the assumption that gas displaces water from capillary-like pathways, with the threshold for gas entry controlled by the capillary entry pressure, requires that the capillary radii (or pore throats) be very small. This gives rise to the large threshold entry pressures reported for highly compacted bentonite. However, a large number of pathways must also then become gas filled to give rise to the observed gas permeability. While such circumstances may be possible, it is difficult to conceive how they would develop in practice.

b) The continuum model of gas pathway propagation with deformation of the clay describes a range of observed phenomena, including pathway resealing and hysteresis through changes in the water content of the clay, although the agreement obtained with experimental data is only of comparable quality to that obtained with the other models.

c) A model that extends a formulation analogous to that referred to in the previous paragraph (b), to include a proper treatment of the interaction of stresses and strains in the clay with gas migration gives comparable agreement in simulations of the same experiment. Work to simulate gas propagation in samples of different geometrical configurations is ongoing.

Experimental data on the mechanism of gas migration in bentonite that allows confirmation of which of the preceding choices of modelling approach is/are most appropriate is currently lacking.

A summary of a major part of the experimental evidence around gas transport in bentonite buffers can be found in /Rodwell 2005/. Results from experiments and modelling from several groups are presented and some conlusions are drawn:

- A threshold pressure for gas entry is observed in many experiments (exception: long term Canadian experiments). The gas entry pressure could be related to the swelling pressure.
- Only small volumes of water are displaced.
- After breakthrough, gas flows at pressures below the threshold, but flow ceases at pressures above back pressure.
- Porewater pressure changes in response to applied gas pressure.
- Evidence for macroscopic fracturing in radial flow experiments.

Although there remained uncertainty in the mechanisms of gas migration in bentonite, it is believed that the research into the subject being carried out in a number of laboratories was satisfactorily addressing the key issues with relevance to the effect of gas generation on the safety performance of bentonite buffers in radioactive waste repositories.

Natural analogues/observations in nature

/Tissot and Pelet 1971/ discuss oil and gas movements in clay shale: "The extraction of oil or gas from a finely structured clay matrix runs contrary to the capillary laws and is in principle impossible. However, the barrier can be broken in one way. The pressure in the fluids that is formed in the pores in the clay increases when kerogen is formed. When this pressure exceeds the mechanical strength of the clay, microchannels will form which are orders of magnitude larger than the natural pores and will thereby allow an oil or gas phase to pass, until the pressure falls below a threshold value and the channels fill again and a new cycle begins." These observations are consistent with the preceding discussions on mechanisms from the gas transport experiments in bentonite.

Time perspective

Gas transport can occur when water is in contact with the cast iron insert in a damaged or breeched (corroded) canister. Unless damaged prior to installation or as the result of some other post-emplacement mechanism, it is unlikely that gas will be released during the first 10,000 years of the repository lifetime.

Handling in the safety assessment SR-Can

Unsaturated conditions: The gas/air quantity in a deposition hole is approximately six percent of the whole volume at atmospheric pressure. When the hydrostatic pressure has been built up, this gas volume will have declined by a factor of 50, at an assumed 5 MPa hydrostatic head. This small quantity is expected to rapidly dissolve in the pore water and can be neglected in the water saturation calculations.

Saturated conditions: The bentonite buffer is an important barrier in the KBS-3 system. The key purpose of the buffer is to serve as a diffusional barrier between the canister and the groundwater in the rock. An important performance requirement on the buffer material is to not cause any harm to the other barriers. Gas build-up from corrosion of the iron insert could potentially affect the buffer performance in three ways:

1. Permanent pathways in the buffer could form at gas break-through. This could potentially lead to a loss of the diffusional barrier.
2. If the buffer does not let the gas through, the pressure could lead to mechanical damage of the other barriers. The main concern is damages to the near field rock.

3. The gas could dehydrate the buffer.
4. A gas phase could push water with radionuclides through the buffer along gas-generated pathways.

The process of gas transport within the buffer is neglected except for deposition holes containing a defective canister. For that case, results of model and experimental studies of gas build-up and transport must be considered in an integrated assessment of the internal evolution of a damaged canister, including corrosion of the cast iron insert and water transport in the canister.

Model: The consequences of gas generation are estimated based on the experimental evidence mentioned above.

Boundary conditions: Gas is generated inside the canister and will be released to the rock through the buffer. Increased total pressure may occur anywhere in the system.

Handling of variables influencing this process: The global rate of corrosion of the insert determines if the hydrogen gas produced can escape by diffusion or if a separate gas phase will be formed. The corrosion rate also determines the rate of pressure increase. This pressure will be transferred to the near-field rock and the backfill. At a certain gas pressure, it is assumed that the buffer will open and let the gas through. This maxium pressure is (probably) dependent on the swelling pressure of the buffer. It is also influenced by the hydrostatic pressure and therefore the effect of a glacial overburden, leading to increased pressures, needs special consideration. The gas pathway in the buffer will stay open as long as the gas production rate is sufficiently high.

The integrated assessment of the internal evolution of a damaged canister will be carried out in the SR-Can Main Rerport.

After repository closure, the only direct flammability hazard to man that could arise is from the release of hydrogen at the surface. This has been assessed and found to be extremely unlikely to present any hazard (the calculation was for release into a building /Baker et al. 1997/). The flammaibilty hazard will not be analyzed in SR-Can.

Uncertainties

Uncertainties in mechanistic understanding

Gas transport: A remaining uncertainty in the understanding of gas transport in the buffer material concerns the number, size and spatial arrangement of the gas-bearing fractures and the volume behaviour of the clay during gas injection. As mentioned in the Experiments/Models section above, the observed gas transport through bentonite can be interpreted in different ways.

One critical uncertainty is the break-through pressure, i.e. the pressure when the buffer opens and lets the gas through. This determines the maximum pressure that can be created within the nearfield of the repository. Another uncertainty is the closure pressure, the pressure where the pathways in the bentonite do close.

These uncertainties will be considered in the integrated assessment mentioned above.

Model simplification uncertainties for the above handling in SR-Can

The evolution of the gas pressure and the gas transport in bentonite in SR-Can is still entirely based on values obtained from experimental results. The uncertainties regarding the interpretation of the experiments make predictive modelling difficult at this stage (see above).

Input data and data uncertainties for the above handling in SR-Can

The maximum gas pressure in the near-field is determined by the break-through pressure in the bentonite. In some experiments, this pressure has been found to be above 20 MPa for a bentonite with a swelling pressure of ~ 6 MPa. The high pressure may be an effect of the small experimental specimen, but since no data from large-scale experiments are available, high breakthrough pressures cannot be ruled out.

Also the gas production (corrosion) rate, which determines the timescale of the gas evolution history, is uncertain.

These data uncertainties will be considered in the integrated assessment mentioned above.

2.3.4 Piping/erosion

Overview/general description

Water inflow into the deposition hole will take place mainly through fractures and will contribute to the wetting of the buffer. However, if the inflow is localized to fractures that carry more water than the swelling bentonite can adsorb, there will be a water pressure in the fracture acting on the buffer. Since the swelling bentonite is initially a gel, which increases its density with time as the water goes deeper into the bentonite, the gel may be too soft to stop the water inflow. The results may be piping in the bentonite, formation of a channel and a continuing water flow and erosion of soft bentonite gel. There will be a competition between the swelling rate of the bentonite and the flow and erosion rate of the buffer.

Piping will take place and the pipes remain open if the following three conditions are fulfilled:

1. The water pressure p_{wf} in the fracture, when the water flow is prevented, must be higher than the sum of the counteracting total pressure from the clay and the shear resistance of the clay.
2. The hydraulic conductivity of the clay must be so low that water flow into the clay is sufficiently stopped to keep the water pressure at p_{wf}
3. There is a downstream location available for the removal of eroded materials in order for the pipe to stay open

Erosion will take place if the drag force on the clay particle from the water movement is higher than the sum of the friction and attraction forces between the particle and the clay structure.

Piping probably only occurs before complete water saturation and homogenisation since the swelling pressure of the buffer material is very high. Erosion can occur both as a consequence of channels caused by piping and over the long-term at the interface between the clay and the fractures in the rock. Since the water flow rate in the latter case is very low, erosion will only be important for colloids leaving the clay gel that has penetrated into the fractures, see further Section 2.5.10. Piping and erosion are thus two completely different processes, but in order for erosion to take place there must be an open channel caused by piping (except for the colloid case).

If piping has occurred it is essential for the function of the buffer that the buffer swells and closes the channel. The ability of the buffer to seal the channel requires the following

1. The mass transport rate of the swelling of the bentonite into the channel must be larger than the mass transport rate of the erosion
2. When the channel has been sealed piping must not occur again (see above).

Influencing/influenced variables

Table 2-8 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Table 2-8. Process/variable table for the process Piping/erosion.

Variable	Does this variable influence the process?		Does the process influence this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Buffer geometry	The distance between the bentonite blocks and the rock surface strongly influences the disposition to piping, since it affects the time to reach a high swelling pressure	The geometry of the buffer is simplified – only a mass balance is used	Yes	Amount of lost buffer is calculated
Pore geometry	Indirect through stress state		Indirect through stress state	
Radiation intensity	No		No	
Temperature	No		No	
Water content	A change in water content changes the swelling pressure, which influences the piping risk. It also influences the hydraulic conductivity, which influences the swelling rate.	Piping will only occur before the buffer is fully saturated	No	
Gas content	No		No	
Hydrovariables (pressure and flows)	Yes	The hydraulic gradient and duration is included in the estimate of piping	Yes	The pipes are assumed to seal when the hydraulic gradients are restored. An "after piping" hydraulic conductivity is estimated
Stress state	Yes	The swelling pressure determines if piping can occur	Yes	An "after piping" swelling pressure is estimated
Bentonite composition	The bentonite and montmorillonite composition affects variables that are important	Indirect through stress state	No	
Montmorillonite composition	The bentonite and montmorillonite composition affects variables that are important	Indirect through stress state	No	
Pore water composition	The salinity of the water affects many variables that are important for disposion to piping and erosion, i.e. the swelling pressure, the swelling rate (through hydraulic conductivity) and the erodability	Pore water composition will affect the amount of eroded buffer. However, a conservative upper limit is used in SR-Can	No	
Structural and stray materials	No		No	

Boundary conditions

The piping and erosion that are treated here only takes place at the interface between the buffer material and the rock.

Model studies/experimental studies

The processes are studied in conjunction with studies for the KBS-3H concept[2], which is particularly vulnerable to erosion of buffer material since a channel can pass close to a large number of canisters. Tests have been done in three different scales. The results show that the bentonite is very sensitive to piping and erosion and that it may take a considerable time until it heals if the inflow in one spot from a fracture is strong and the build-up of water pressure in the fracture is fast. See /Börgesson et al. 2006/.

The phenomenon has been observed in two field tests in Äspö HRL (LOT /Karnland et al. 2000/ and in the full scale test Lasgit). One of the deposition holes in the Prototype Repository has a rather large water inflow and may be used as a check of one scenario for piping erosion. However, this section of the test is not planned to be excavated for at least another 10 years.

Natural analogues/observations in nature

Not applicable for this process.

Time perspective

The piping and erosion (excluding colloid erosion) only takes place before complete saturation and homogenisation. The high swelling pressure of the buffer will ultimately seal the piping channels, since the sum of the swelling pressure and the pore water pressure in the buffer will always be higher than the water pressure. The water inflow must though not be so strong that the buffer has lost too much bentonite through erosion.

Handling in the safety assessment SR-Can

Model: The maximum consequences of this process will be estimated by model calculations. This will be based on the experiences from the KBS-3H study.

Time periods: The piping/erosion process is only relevant during saturation and is neglected for all other time periods.

Boundary conditions: The hydraulic boundary conditions at the buffer/deposition hole interface are decisive for this process.

Handling of variables influencing this process: The water flow and the water pressure together with the water pressure increase rate are the key variables for this process. The erosion is also affected by the geometry of the initial slots in the system. The effect of the salinity of the groundwater is also included in the description.

Handling of variables influenced by the process: The consequence of an extensive piping together with erosion would be a loss of buffer density.

The special cases of failed canister and of earthquakes: The process only occurs at very early stages when these special cases are not relevant.

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[2] In the KBS-3H concept, canisters are deposited horizontally in long tunnels, rather than vertically in individual deposition holes.

Uncertainties

Piping, erosion and subsequent sealing is a complicated process with many components, much depending on the hydraulic behaviour of the rock. The uncertainties are considerable regarding both the demands on the rock and the ability of the buffer to resist these processes. For the KBS-3H concept, a preliminary demand is that one canister position must be able to handle the inflow 0.1 l/min and a pressure increase of the water pressure in a fracture intersecting the tunnel of 100 kPa increase per hour. This could thus be transferred to demands of the deposition hole, but it is not obvious that the demands should be equal. Furthermore, the time required for the buffer to seal such an inflow from a fracture is not known.

The knowledge of when piping and erosion occur and the consequencies are not enough known today. Further tests are ongoing and planned.

2.4 Mechanical processes

2.4.1 Swelling/mass redistribution

The swelling process has been merged with other stress-strain-related processes that can cause mass redistribution within the buffer, namely thermal expansion, creep and a number of interactions with the canister, near field rock and the backfill.

Overview/general description

Water is absorbed by both unsaturated and saturated bentonite (that is able to physically expand) and causes swelling. If the bentonite is unable to expand freely, a swelling pressure develops, which locally reaches its peak at full water saturation.

In a deposition hole the buffer is inhomogeneous from start due the slots at the horizontal buffer boundaries. When water from the rock fills the outer (potentially pellet–filled), slot and enters the bentonite blocks there will be swelling of the blocks and compression of any pellets located in the outer slot. At first the swelling will be strong since the overall density of the pellet-filled slot is low and the resistance against compression thus small relative to that of the buffer. This means that the outer part of the blocks will swell to a lower density than the average density expected after complete homogenisation. Ultimately the water will be drawn so deeply into the blocks that the swelling pressure compresses both the pellet-filled gap and the swollen outer part of the blocks. With time after saturation is achieved, the compression of the outer part and the expansion of the inner part will come to some kind of equilibrium. This will not likely be a completely homogenous material due to inner friction in the bentonite and hysteresis effects. A small density gradient is expected to persist with higher density close to the canister and lower close to the rock will endure.

The swelling also leads to compression of the backfill above the deposition holes, a mechanical pressure on the canister and rock surface of the deposition hole, and clay intrusion in fractures around the deposition hole. Depending on the conditions in the near-field rock, the clay in the fractures could be carried away by the groundwater (under conditions of high local groundwater flow through the fracture(s)), allowing new clay to penetrate. This could lead to gradual erosion of the buffer (see Section 2.5.10). Besides themechanical effects, the buffer's hydraulic conductivity and diffusion properties are also altered by swelling.

Other phenomena that could lead to mass redistribution, expansion or contraction of the buffer include creep, shear movements and convergence of the deposition hole, canister movements, pressure exerted by canister corrosion products and thermal expansion of the buffer pore water.

The following description illustrates the principles adopted for modelling of swelling from a geotechnical perspective. This approach does not address the underlying mechanisms that control the behaviour.

The swelling can be conceived of as being caused by a force of repulsion between the montmorillonite layers. If there is a limited supply of water in a free specimen, the swelling is counteracted by a negative pressure in the pore water. If a specimen is water-saturated, i.e. all pores are filled with water; the swelling is counteracted by the formation of a negative pressure in the pore water in the water menisci on the surface of the specimen. The negative pore pressure is equal to the internal swelling pressure if no external pressure is applied. If the specimen is unsaturated, the water menisci develop inside the specimen as well. The negative pressure in the pore water is chiefly a function of the water ratio in the specimen, i.e. the quantity of water per unit weight of dry material. This negative pressure is called suction potential (see also Section 2.3.1). When water is added to an unconfined specimen, the water ratio increases, and the repulsion forces and the suction potential decrease. This causes the specimen to swell until a new equilibrium is established with a lower internal swelling pressure. If the volume is kept constant, a portion of the internal swelling pressure is instead transferred to an external swelling pressure, which can be measured. When a specimen with constant volume is completely water-saturated and the pore water pressure is kept positive, the entire swelling pressure becomes an external pressure. At water saturation, the swelling pressure and the pore water pressure are independent quantities and give a total pressure that is the sum of the pressures.

Table 2-9 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

The data and discussion on influences in the following text are in principle valid for MX-80 but the mechanical properties of Deponit CA-N bentonite is similar to the properties of MX-80, which means that they can also be applied to Deponit CA-N bentonite.

Measured swelling pressure at constant volume after water saturation is shown in Figure 2-7 and Figure 2-8 for both MX-80 and Deponit CA-N bentonites /Karnland et al. 2005/. The influence of density and ion concentration in the saturating water is measured and included in the figures.

Influence of density: The density at water saturation is decisive for the water ratio, which determines the swelling pressure. Figure 2-7 and Figure 2-8 illustrate the difference in swelling pressure at different densities.

Influence of montmorillonite content and species of adsorbed cation: According to Figure 2-7 and Figure 2-8, the swelling pressure is relatively independent of the adsorbed ion is sodium or calcium if the density exceeds approximately 1,800 kg/m^3 and the montmorillonite content are the same. At lower densities the swelling pressure is lower if the adsorbed ion species is Ca. Reduced montmorillonite content can be conceived of as being equivalent to the addition of an inactive aggregate (ECDD/EMDD, see Table 1-7) and the influence is best expressed with the effective montmorillonite dry density (dry mass of montmorillonite divided with the net volume (the total volume minus the volume taken by the non-montmorillonite particles)).

Influence of chemical composition of pore water: Increased ion concentration generally leads to a reduced swelling potential, and thereby to effects on the pore geometry that are similar to those of an ion exchange to divalent ions. Increased ion concentration further leads to a reduction of the swelling pressure due to osmotic effects, and to changes in the pore geometry that affect the hydraulic conductivity of the material at low saturated densities (< 1,800 kg/m^3) (see Section 2.5.8).

Influence of degree of saturation: In an unsaturated state, the bentonite/water system shrinks on drying and expands on wetting. The volume change on water uptake in e.g. a block is less in the unsaturated state, since the swelling takes place partially in previously unfilled pores. Shrinking due to drying is expected to take place near the canister, which can lead to cracking of the buffer. After full saturation the cracks will be healed and the buffer homogenised in the same way as all initial slots and joints between blocks in a deposition hole.

Table 2-9. Process/variable table for the process Swelling/mass redistribution.

Variable	Does this variable influence the process?		Does the process influence this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Buffer geometry	Any phenomenon leading to alterations of the buffer bulk geometry influences swelling	The initial position of the buffer is the starting point of the evaluation	Yes	The buffer geometry after swelling is estimated
Pore geometry	Indirectly through stress state		Indirectly through stress state	
Radiation intensity	No		No	
Temperature	Through thermal expansion	Excluded from assessment (see below)	(Insignificant)	
Water content	Yes	Included in THM modelling of unsaturated buffer	Yes	Included in THM modelling of unsaturated buffer
Gas content	Degree of saturation	Included in THM modelling of unsaturated buffer	Degree of saturation	Included in THM modelling of unsaturated buffer
Hydrovariables (pressure and flows)	Yes	Included in THM modelling of unsaturated buffer	Yes	Included in THM modelling of unsaturated buffer
Stress state	Yes	Included in THM modelling of unsaturated buffer Is included in calculation of the mechanical interaction with the canister as well as backfill	Yes	Included in THM modelling of unsaturated buffer Is included in calculation of the mechanical interaction with backfill
Bentonite composition	Yes	The initial composition of the buffer is the starting point of the evaluation	No	
Montmorillonite composition	Yes	The initial composition of the buffer is the starting point of the evaluation	No	
Pore water composition	Yes	The swelling pressure is given from the porewater composition	No	
Structural and stray materials	Yes	Not considered with the SR-Can assessment	No	

If volume is restrained during water uptake, which is the case for the buffer in a deposition hole, the expansion will be replaced by a swelling pressure that gradually increases as the degree of saturation increases. If there is a difference or gradient in degree of saturation the pressure in a less saturated part can be higher due to transmission of pressure from more saturated parts.

Influence of temperature: A change in the temperature of the buffer will cause water, particles and pore gas in the buffer to expand and may influence the mechanical properties of the buffer.

The influence of temperature on the mechanical properties of the buffer in the water-saturated state is small /Börgesson et al. 1995/. In the unsaturated state, this influence is presumably small /Villar 2002/ but is not sufficiently well-known for MX-80.

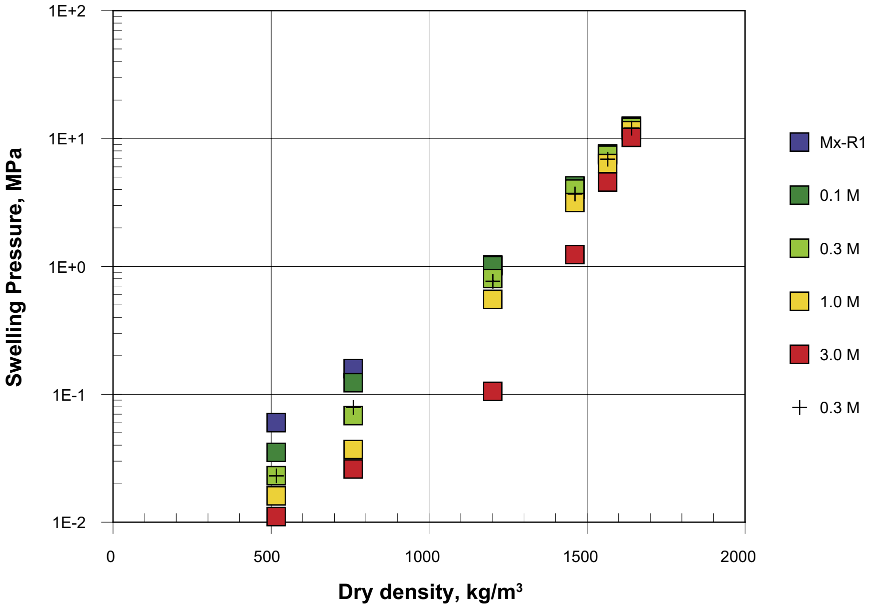

Figure 2-7. *Swelling pressure of MX-80 bentonite measured at different densities and molar concentration of NaCl in the saturating solution All tests have been performed with increasing salt concentration except for the tests denoted +, which have been performed after reduction in salt concentration from 3 molar.*

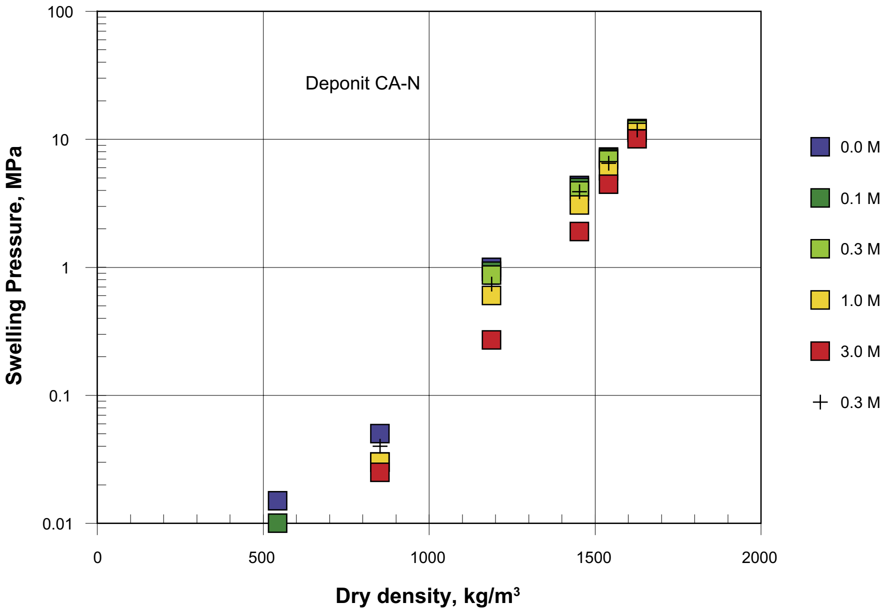

Figure 2-8. *Swelling pressure of Deponit CA-N bentonite measured at different densities and molar concentration of* $CaCl_2$ *in the saturating solution. All tests have been performed with increasing salt concentration except for the tests denoted +, which have been performed after reduction in salt concentration from 3 molar.*

The expansion of the particles and the pore gas is relatively small. The expansion of the water, which is about 100 times greater than the expansion of the particles, completely dominates this process.

The influence of the water's expansion is completely dependent on whether the buffer is water-saturated or not. Before water saturation the volume of the water can expand with virtually no other resistance than that offered by the compression properties of the pore gas. At constant volume this leads (to simplify slightly) to an increase in the degree of saturation when the temperature increases. The consequences of this are that the negative pressure in the pore water (suction potential) decreases and that the total pressure and the pore gas pressure increase. This causes the swelling pressure against an external restraint to increase slightly. At constant pressure, a slight increase of the volume is obtained in the same way. However, these changes are small and apparently without practical significance. The increase in degree of saturation is about 2 percent at a temperature increase of 50 degrees.

The consequences can be more serious in water-saturated buffer, since there are no gas-filled pores to accomodate the volume increases of the solid and liquid components. At constant volume the pore pressure increase is great since the water is unable to expand. Theoretically, the resultant pressure increase against the surroundings can amount to several tens of MPa at the temperature changes in question. However, the pressure increase is counteracted by drainage of the water through the rock and backfill. This causes a moderation in the magnitude of the pore pressure increase that would otherwise occur in parallell with the temperature increase. This process of excess pore pressure dissipation can be relatively fast and can greatly reduce the pore pressure increase if the temperature increase is slow and a drainage path is available.

Boundary conditions

The boundary conditions of interest mainly concern alterations of the geometry of the buffer's interfaces to the near field rock, to the canister and to the deposition tunnel backfill.

Interaction buffer/backfill

In the interface between the buffer and the backfill, the buffer exerts a swelling pressure against the backfill and vice versa. Since the difference in swelling pressure may be great, a net pressure arises against the backfill whereby the buffer swells and the backfill is compressed. In this process, the swelling pressure from the buffer decreases as the density decreases. At the same time, the counter-pressure from the backfill increases as it is compressed and its density increases. The swelling of the buffer and compression of the backfill are counteracted to some extent by friction against the rock. When the force of the swelling pressure in the buffer is equal to the sum of the force of the counter-pressure in the backfill and the friction against the rock, the process ceases since equilibrium has been established.

The size of the swelling pressures generated depends on the original densities of the buffer and the backfill and associated expansion and compression properties.

Due to the friction against the rock and friction in the buffer, the homogenization of the buffer is not complete. When the buffer swells upwards due to compression of the backfill the friction in the buffer leads to an axial gradient in swelling pressure and density. The density increases with increasing distance from the interface and reaches ultimately the average density at some distance. For typical densities in the backfill (30/70) this distance with reduced density does not reach down to the canister, which lies 1.5 m below the interface.

Figure 2-9 illustrates the displacement of the interface between the buffer and backfill and the displacement of the canister as a result of a finite element calculation of the wetting of the buffer for a rock with one fracture intersecting the centre of the deposition hole. /Börgesson and Hernelind 1999/. The results show that the buffer/backfill interface heaves about 8 cm. The upwards swelling also affects the canister before full saturation of the buffer. The canisters at first heaves 5–10 mm due to the uneven wetting of the buffer but settles at the completion of the wetting and ultimately reaches its initial position. The results also show that after full saturation and completed consoidation the density and swelling pressure are reduced above the canister but not along the sides of the canister.

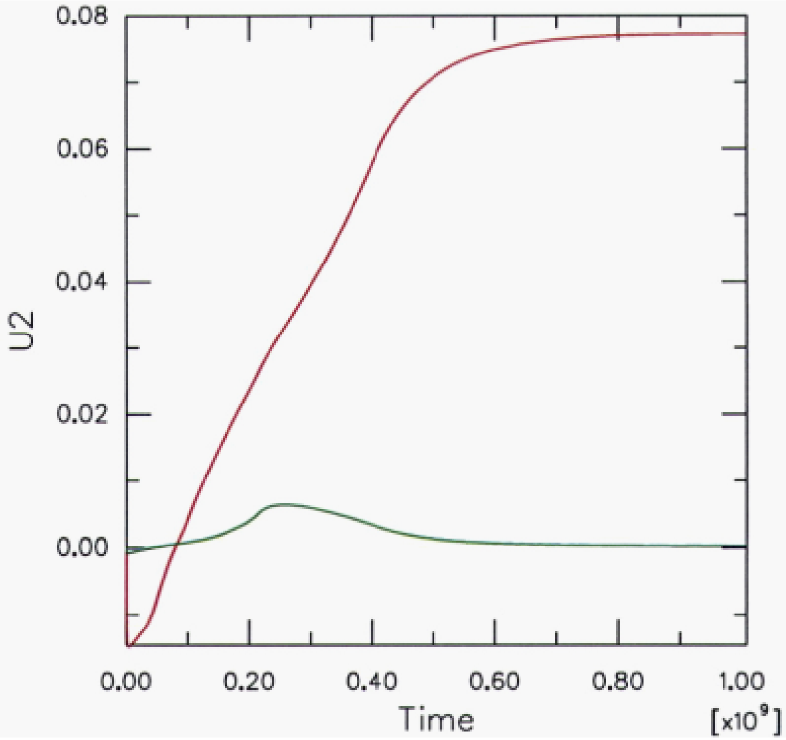

Figure 2-9. *Heave (m) of the buffer/backfill interface (red) and the canister (green) as a function of time (s) elapsed from deposition. Example from a FE-calculation.*

Interaction buffer/near field rock

The following mechanical interactions between buffer and near-field rock have been identified:

1. **Swelling pressure from the buffer** is transferred to the rock but is not expected to lead to significant rock movements. The elastic deformation of the rock at the expected swelling pressures is small due to the rock's high modulus of elasticity. Plastic deformations caused by movements along a fracture plane can occur along rock wedges that go up to the tunnel floor. The swelling pressure also reduces the ongoing rock stress release (from the rock excavation) and the extention of the damaged rock zone adjacent to the deposition hole (see the geosphere process report).
2. **Pressure from the canister** can be propagated via the buffer. Such pressures can arise from canister corrosion products and gas pressure build-up.
3. **Forces of friction** arise against the rock walls in the deposition hole due to swelling of the buffer against the backfill.
4. **Thermal expansion of the buffer** can be serious for the rock if the buffer is water-saturated when the temperature increase occurs. This process is described above. The slow temperature increase in combination with the drainage through the rock implies that this is not a problem but it should be checked by some calculations. If the rock is very tight the drainage could be hindered, but such a rock will not provide enough water to yield saturation before the peak of the thermal pulse.
5. **Convergence of the deposition hole** occurs when the rock creeps due to the high rock stresses after rock excavation. Assuming an anisotropic primary state of stress with reasonable components, calculations have shown that the diameter can decrease by approximately a centimetre after 10,000 years /Pusch 1995/. The resulting density increase in the buffer leads to an increase in the swelling pressure by roughly a few MPa. Recent conservative estimates of creep-induced deformations of deposition tunnels have given convergence values of

about 1% /Glamheden et al. 2004/. For a deposition hole this would give between 1 or 2 cm of diameter reduction. The recent estimates are based upon the notion that creep will relax fracture shear stresses over time until a low threshold stress has been reached. The effect can be even greater at higher rock stresses, caused by e.g. glaciation.

6. **Shear movements due to sliding** along a fracture in the rock is a process that can be serious for the canister if the displacement is rapid and great. The process is partially dealt with below (Interaction buffer/canister). Rock movements are dealt with in the forthcoming process descriptions for the geosphere, see the Process report for SR 97 /SKB 1999/ for an earlier description.
7. **Intrusion of bentonite into fractures in the rock** is very limited due to the small aperture of the fractures and the shear resistance caused by the friction between the bentonite and the fracture surface. If there is no loss in bentonite due to erosion the effect is positive since it implies a sealing of the fracture. Problems may occur if the gel that forms at the outer part of the penetrated bentonit is eroded and carried away by the groundwater.

The depth of the intrusion is a function of the fracture width, the friction between the bentonite and the rock surface and the swelling pressure in the deposition hole. The penetration depth z can be calculated according to the Equation 2-11 (derived from simple integration of force equilibrium):

$$z = \frac{\delta}{2\tan\phi}\left(\ln\sigma_0 - \ln\sigma_z\right) \qquad \text{(2-11)}$$

where

δ = fracture width

φ = friction angle (10–30 degrees)

σ_0 = swelling pressure on the rock (7–13 MPa)

σ_z = swelling pressure in the fracture at the distance z from the rock surface

The penetration depth will thus go towards infinity when the swelling pressure at the gel limit approaches 0. If the swelling pressure 1 kPa is set as a limit the penetration from a buffer with the swelling pressure 10 MPa into a fracture with the width 0.1 mm will be 1.3 mm if the friction angle 20 degrees is assumed (an average). If the limit pressure 1 Pa is set the penetration will be 2.2 mm. Extrapolating the swelling pressure relations (not verified) one finds that 1 kPa corresponds to the void ratio e=70 (w=2,500%) for fresh water and e=3.5 (w=125%) for sea water.

The effective stress can never be less than the self weight of the gel. This stress can thus be used to find the minimum pressure σ_z in Equation 1. At the salt content 0.6%, which is relevant for Swedish repository conditions, the maximum swelling capacity of MX-80 is swelling to a water ratio of 215% /Wold 2003/. This corresponds to a density at saturation of 1,250 kg/m^3. For a horizontal fracture of 0.1 mm width the effective stress on the “bottom” of the fracture from the self weight of the gel will thus be 0.25 Pa, which yields an average effective stress of 0.125 Pa that the gel never can pass. If this limit is applied the penetration will be limited to 2.5 mm.

Since the penetration depth is proportional to the fracture width a rule of thumb may be that the penetration is limited to 25 times the fracture width.

This process is also dealt with in Section 2.5.10.

General comments

The influence of the buffer on the rock is difficult to investigate experimentally in any other way than by measuring the swelling pressure on the rock. This has been done in BMT in Stripa /Pusch et al. 1985a/ and in several of the full-scale tests in Äspö HRL /Goudarzi et al. 2003/. Calculations of the effect on the rock of corrosion of the cast iron insert show that the influence is small /Bond et al. 1997/. The effect on the rock of the buffer's upward swelling in the deposition hole has been modelled /Pusch and Börgesson 1992/. These studies show that a rock wedge can, if the backfill is poorly compacted, move upward 0.2–0.3 m and reduce the density of the buffer in the upper part of the deposition hole. This scenario presumes that a triangular wedge reaches from the floor in the tunnel more than a meter down to the buffer in the deposition hole. It also presumes that the wedge is attached to the rock during installation of the buffer and backfill but detached either during compaction of the backfill or due to thermal stresses (or similar) after deposition. The swelling pressure and the axial upwards swelling of the buffer can then move the wedge upwards and create an increased volume of the deposition hole. This combination of events has thus been considered but is very unlikely.

The influence of the rock on the buffer in connection with shear movements along fracture planes has been studied in both experimental and model studies. This process is not harmful for the buffer (if its rheological properties have not been changed) but only for the canister (see below).

Processes 1, 3, 4 and 7 listed above are most likely to occur during the first 100 years after closure of the repository. The other processes occur or can occur throughout the lifetime of the repository.

The uncertainties concerning processes 1–4 and 6 stem mainly from uncertainties in other processes and are dealt with elsewhere (canister corrosion, gas formation, canister/buffer interaction, etc).

Convergence of the deposition holes is normally negligible.

The penetration of buffer into fractures is of no importance for the buffer unless followed by erosion. This process is treated in Section 2.5.10.

Interaction buffer/canister

Mechanical interactions between the buffer and the canister arise from the buffer through the clay matrix. Both compressive stresses and shear stresses are generated in the clay. The pore water and gas within the buffer will generate only compressive stresses. Changes in these three factors take place during the water saturation process and can also occur in response to external forces. The weight of the canister influences the buffer, while the influence of the weight of the buffer on the canister is negligible.

The mechanical interaction between buffer and canister is summarized in the following 7 processes:

1. Swelling pressure and water pressure exerted on the canister.

The magnitude of the swelling pressure is described above. During the saturation process the swelling pressure may be uneven mainly due to uneven wetting, but after full saturation the swelling pressure is rather homogeneous. The water pressure is added to the swelling pressure to give the total pressure the surface of an intact canister will experience and is also uniform with the expected magnitude given by the depth of the repository. During glaciation the water pressure may be substantially higher.

2. Thermally induced pore water pressure exerted on the canister.

This process is described above. The process can be detrimental for the canister if the following two criteria are fulfilled:

1. The buffer is water saturated during increasing temperature
2. The water volume decrease caused by the pressure reduction during drainage of the water through the buffer out to the rock and backfill is slower than the water volume increase caused by the thermal expansion of the water during the increasing temperature.

Preliminary calculations have shown that the latter criterion is not probable /Pusch and Börgesson 1992/. The first criteria above may be fulfilled but is not enough on its own for causing high pore pressure and requires the second in order to become an issue.

3. Trapped gas in the buffer exerts pressure on the canister.

Gas generation is treated in Section 2.3.3. High gas pressures are only expected as a possible consequence of corrosion of the insert of a failed canister. In that case, the gas pressure will act on both the inside and the outside of the canister and the net mechanical effect on the canister should thus be negligible.

4. Canister corrosion products exert pressure on the canister.

External corrosion of the copper canister and corrosion of the steel insert in the case of a defective copper canister, will increase the volume of the canister since the corrosion product has a lower density than the original material. This material expansion will result in compression and consolidation of the buffer and thereby increase the pressure from the buffer on the canister. This process will be further treated in the forthcoming reporting of canister processes.

5. Vertical movement of canister in buffer.

The average density of the canister is much higher than that of the buffer, which means that there is a net vertical stress on the bottom part of the buffer in the deposition hole. This stress difference results in a density that is slightly higher below the canister than in the other parts of the buffer. This means that there is a net vertical sinking of the canister in relation to the original location. On the other hand, there is an upward swelling of the buffer above the canister (due to the compression of the backfill; see above), resulting in a decreased density and decreased swelling pressure above the canister. This may lead to a swelling pressure below the canister that is higher than the sum of the weight of the canister divided by the cross sectional area and the swelling pressure on the top of the canister. Since the upward-directed force on the canister will therefore be higher than the downward-directed force, the canister will heave instead of sink.

There is thus a complicated combination of pressure (and forces) on the canister. The result can be calculated and leads to equilibrium after complete water saturation and pore water pressure stabilisation, which includes stress differences and shear stresses in the buffer. This equilibrium is typically established within 100 years after closure of the repository whereupon creep phenomena will dominate the displacements in the buffer.

There are three types of time dependant displacements of the buffer resulting in movements of the canister. One is related to what in soil mechanics is named “primary consolidation”, the second one to so called “secondary consolidation” (volumetric creep) and the third to time dependant shear deformations (deviatoric creep).

During primary consolidation the pore water pressure is the regulating variable and the time perspective is determined by the hydraulic conductivity and the compression properties. Before equilibrium in effective stresses in the clay skeleton is established, the pore water carries the total pressure difference. With time, as the pore water pressure difference is reduced due to outflow of water, the pressure induced by the canister mass is transferred from the pore water to the clay skeleton and the clay is thus deformed. This process dominates as long as there are pore water pressure differences in the buffer.

After pore pressure equilibrium the creep processes dominate. The volumetric creep is caused by internal microstructural reorganization of the clay particles and is related to the change in swelling pressure with time. This creep is not particularly large in buffer and backfill materials and not problematic as far as vertical movements of the canister are concerned, since it will not remove any bentonite but (in the case of constant stress) only compress it or (in the case of constant volume) relax the stresses.

The deviatoric creep is potentially problematic since the existence of deviatoric stresses (or shear stresses) is dependant on internal friction or cohesion in the clay. These parameters are slightly reduced with time, which causes a deviatoric creep and thus a movement of the canister. If the friction and cohesion are reduced to zero the clay would behave as a viscous liquid and there would be no resistance against the canister sinking to the floor of the deposition hole.

The deviatoric creep has been investigated with a number of creep tests at different stresses and a creep model has been derived /Börgesson et al. 1995/. The model has been used in preliminary finite element calculations. The calculations were actually made on the concept with two canisters in a deposition hole but the results are also applicable for the reference concept with one canister. They show that the creep settlement after water saturation is a few mm in 300 years and less than a cm if extrapolated to 100,000 years /Börgesson 1993b/. Similar creep settlement has been found by use of a quite different approach based on creep theory of stochastic mechanical origin /Pusch and Adey 1999/.

Present studies of deviatoric creep aim at establishing a critical buffer density, such that if the density exceeds the critical value, canister sinking can be ruled out (see below).

6. Transfer of shear stresses from rock via buffer to canister, especially during an earthquake

An earthquake may induce a shear displacement along a fracture that intersects a deposition hole. The rock displacement will pressurise the bentonite in the deposition hole on the active side and cause high shear stresses that lead to plastication in the area between the fracture and the canister. The pressure on the active side will be transferred to the canister and make the canister partly tilt and partly be bent.

The effect on the canister is depending on the stiffness or shear strength of the bentonite in relation to the stiffness of the canister. The shear strength of bentonite is dependant on the density and the rate of deformation. This scenario has been thoroughly investigated recently and is described under “Model studies” below.

7. Intrusion of buffer in a damaged canister

Bentonite may penetrate into a damaged canister. The influence on the buffer is though small due to the small void available inside the gap between the copper and the insert.

Model studies/experimental studies

Saturated bentonite

Bentonite’s swelling capacity and swelling pressure under water-saturated conditions has been studied in detail by means of laboratory experiments /Börgesson et al. 1995/. The results have been used to devise a material model that can be used for FEM calculations /Börgesson et al. 1995/. It is based on the effective stress theory and coincides largely with models for other soils, although the magnitude of the swelling and pressure are considerably greater for bentonite.

The material models have been used to calculate different evolutions that are associated with volume changes in a repository. Examples of modellings are the following:

- Swelling of buffer against the backfill in deposition holes /Pusch and Börgesson 1992/. A calculation of an extreme case was performed for PASS /Pusch and Börgesson 1992/ where the buffer was assumed to have a density of 2,100 kg/m^3 after water saturation and the density of the backfill was assumed to be 1,900 kg/m^3 after water saturation, which corresponds to higher density in the buffer and lower in the backfill than is stipulated in the reference case /Bäckblom 1996/. This gave an upward displacement of about 30 cm.

- The thermo-hydro-mechanical calculations of the water saturation phase of a deposition hole with different hydraulic rock properties, done for SR 97, included the displacement of the buffer/backfill interface and the movements of the canister /Börgesson and Hernelind 1999/. The average density of the buffer after saturation of 2,000 kg/m^3 and an E-modulus of the backfill of 30 MPa resulted in a heave of the backfill interface of 7–8 cm and a temporary heave of the canister of about 1 mm.
- Settlement experiment in Stripa /Börgesson 1993a/. Comparisons of calculated and measured movements and densities when canisters are loaded in deposition holes.
- Modelling of canister movements for design with two canisters in a deposition hole /Börgesson 1993b/. In conjunction with studies of the function of deposition holes with two canisters, a calculation was made of the movements of the canisters which included upswelling towards the backfill /Börgesson 1993b/. In this calculation the buffer was defined to have a high density (2,100 kg/m^3 at saturation) and the backfill was assumed to be rather stiff, with a density after water saturation of 2,200 kg/m^3. The calculated upswelling of the buffer was about 7 cm and the total heave of the canister (including both cosolidation and creep) after 3,2000 years was 3 mm.
- For a rock shear the influence of the density and the rate of rock displacement has been investigated for very fast shearing and reported recently /Börgesson et al. 2004b/. The influence is illustrated with the following examples: At the density 2,000 kg/m^3 at water saturation the shear strength is 1 MPa at the shear rate $5 \cdot 10^{-8}$ m/s (4 mm/day) while the shear strength is 3 times higher (3 MPa) at the shear rate 1 m/s. At the density 2,100 kg/m^3 at water saturation the shear strength is 2.6 MPa at the shear rate $5 \cdot 10^{-8}$ m/s (4 mm/day) while the shear strength is also at this density about 3 times higher (7.6 MPa) at the shear rate 1 m/s.
- A material model has been established and the effect of rock shear on the canister and buffer calculated. The influence of density, shear rate, magnitude of shear displacement and location of the shear plane has been investigated with finite element modelling /Börgesson et al. 2004b/. The results show that there may be strong plastication both of the copper canister and the steel insert but that the plastic strain is limited to a few percent at the reference case (density 2,000 kg/m^3, shear rate 0.1 m/s, shear displacement 10 cm).

  The maximum plastic strain in the steel insert, after a shear displacement of 10 cm at the density 2,100 kg/m^3, is about 9%, which does not yield rupture of the steel but should anyhow be considered an upper limit. The buffer material should thus not have a density higher than 2,100 kg/m^3 in order to avoid damage to the canister in case of an earthquake.

Recently the vertical displacement of the canister in the KBS-3V concept has been studied in a number of consolidation and creep calculations using the FE-program ABAQUS. The creep model used for the calculations is based on Singh-Mitchell's creep theory, which has been adapted to and verified for the buffer material in earlier tests. A porous elastic model with Drucker-Prager plasticity has been used for the consolidation calculations. For simplicity the buffer has been assumed to be water saturated from start.

In one set of calculations only the consolidation and creep in the buffer without considering the interaction with the backfill was studied. In the other set of calculations the interaction with the backfill was included for a backfill consisting of an in situ compacted mixture of 30% bentonite and 70% crushed rock. The motivation to also study the behaviour of the buffer alone was that the final choice of backfill material and backfilling technique is not made yet so that set of calculations simulates a backfill that has identical properties with the buffer. The two cases thus represent two extremes, one with a backfill that has the lowest allowable stiffness and one that has the highest possible stiffness.

The base cases in the calculations correspond to the expected swelling pressure of 7 MPa in a buffer with the final average density at saturation of 2,000 kg/m^3. In order to study the sensitivity of the system to loss in bentonite mass and swelling pressure seven additional calculations were done with reduced swelling pressure down to 80 kPa corresponding to a density at water saturation of about 1,500 kg/m^3.

The calculations included two stages, where the first stage models the swelling and consolidation that takes place in order for the buffer to reach force equilibrium. This stage takes place during the saturation phase and the subsequent consolidation/swelling phase. The second stage models the deviatoric creep in the buffer during 100 000 years.

The volumetric creep is not modelled, which thus may cause a slight underestimation of the canister displacement. The motive for excluding volumetric creep is that a canister settlement caused by volumetric creep will not change the total mass of bentonite under the canister but will only increase the density and is thus not judged to be a problem. Moreover, the volumetric creep is of the same order of magnitude as the deviatoric, which means that the canister displacement caused by this creep will be as insignificant as the deviatoric creep.

The calculations show that the canister settlement is very small even at low swelling pressure and density. The base case corresponding to the expected final swelling pressure of the buffer 7 000 kPa yields a total settlement of the canister of only 0.35 mm for the fixed boundary case, while there is a heave of the canister of about 4.5 mm at the other case with 30/70 backfill due to the upwards swelling of the buffer. At reduced swelling pressure the settlement increases but is not more than about 23 mm at the very low swelling pressure 80 kPa for both cases.

Figure 2-10 shows the consolidation and creep settlement as a function of applied swelling pressure for the two sets of calculations.

Another phenomenon that may affect the buffer is a reduction in strength or friction angle with time, which affects the degree of mobilized shear strength, which is a critical creep parameter. A reduced friction angle will reduce the strength and thus affect the degree of mobilized strength in a similar way as a reduced swelling pressure. So the reduction in shear strength can for the creep also correspond to a reduction in friction angle with kept initial density and swelling pressure. At the swelling pressure 80 kPa the deviatoric stress at failure is only 70 kPa, which for the swelling pressure 7 000 kPa corresponds to a friction angle of only 0.29 degrees. This shows that not even a strong reduction in friction angle is a threat to the canister integrity.

The conclusion is thus that the expected displacement of the canister in a deposition hole from consolidation and creep during 100 000 years is very small and for the case of 30/70 backfill actually will result in a heave of the canister. The sensitivity analyses with reduced swelling

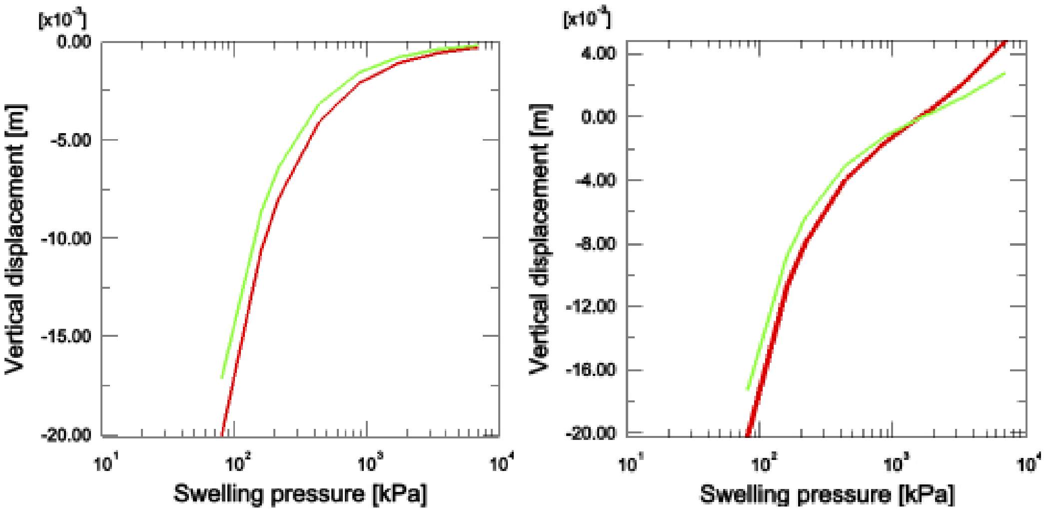

Figure 2-10. *Vertical displacement of the canister as a function of swelling pressure for the two cases with fixed boundary buffer/backfill (left) and free boundary with 30/70 backfill (right). Negative displacement implies sinking.*

🟩 *Only consolidation*

🟥 *Consolidation + creep*

pressure corresponding to reduced density or reduced friction angle also show that the canister displacement is very insensitive to such phenomena since the total settlement will be less than a few cm even at a buffer density of 1,500 kg/m^3 or at a friction angle of 0.3°.

Experience related to swelling and homogenisation of the b uffer in an emplacement borehole is available from the results of field tests in Stripa. In BMT (Buffer Mass Test), six deposition holes were simulated on half scale. The movement of the interface between the buffer and the backfill was measured with a coin that was placed in the interface and levelled before and after the tests. The measured upwards swelling varied between 4 and 7 cm, depending on test time and degree of saturation in the buffer.

Further information related to the homogenisation of the buffer and the mechanical interaction between buffer and backfill is also being collected from several of the full-scale tests in Äspö HRL. One of these, the Canister Retrieval Test is expected to be have achieved full water saturation in the majority of its buffer volume at the time of its excavation, which is planned to take place at the end of 2005.

Several scale tests have been run in the laboratory (mostly in the scale 1:10) to complete water saturation. Two examples of the types of tests conducted are:

- Rock shear was simulated in the scale 1:10 in three laboratory tests performed 1986 /Börgesson 1986/. Before the shear was simulated the bentonite was brought to complete water saturation through filters in the periphery of the buffer and the swelling pressure measured. The three tests were identical with exception of the shear rate that was varied between 0.03 mm/min. to 160 mm/min. The bentonite was carefully sampled and the water ratio and density of the samples were determined after finished test. The tests gave valuable information about both the effect of shear at different rates and the homogenisation of the bentonite in a deposition hole.
- The KBS-3H concept has been simulated in the laboratory also in the scale 1:10. Two canisters with buffer material, perforated steel containers and distance plugs were installed in a tube and mainly the swelling pressure and relative humidity RH were measured. By measuring RH the total suction of the clay and the resulting degree of saturation can be evaluated. The bentonite was brought to complete water saturation through filters with an increased water pressure of 1 MPa. The test arrangement was left for one year and the axial hydraulic function of the buffer was tested by applying hydraulic gradients in the filters. Finally the test was terminated and water ratio and density measured after comprehensive sampling. The test was used to evaluate the swelling and homogenisation of the distance blocks and the buffer inside the perforated container and to study the resulting axial water flow properties. The results showed satisfactory agreement with expectations.

No heating was applied to the two tests described above.

Unsaturated bentonite: Experiments have been conducted to study the volume change as a function of degree of saturation and void ratio. These experiments have been used to calibrate the material model for unsaturated clay.

The interaction between external stress, pore water pressure (suction) and degree of saturation in an unsaturated bentonite has been investigated in a PhD project /Dueck 2005/. This work sheds further light on the development of swelling pressure in an unsaturated buffer. A laboratory programme was run with the ultimate purpose to investigate the influence of confinement on the water retention properties, the development of swelling pressure during decrease in suction and the effect of external load and swelling pressure on suction.

The results from the laboratory tests were used to find a relationship between water content, void ratio, swelling pressure and suction. Two equations for swelling pressure represent the outline of the model. In the first of the equations, the swelling pressure developed during water uptake is normalised by a pressure corresponding to the swelling pressure at saturation. This is done in order to be independent of void ratio. A relationship between the normalised swelling pressure and the degree of saturation is suggested. The second equation describes a relationship between the swelling pressure, the water content and the actual suction (or relative humidity). The equation is based on a thermodynamic relationship and includes the retention curve (i.e. water content vs. suction under free swelling conditions). The model can be used for a state where two of the four parameters; water content, void ratio, swelling pressure and suction are known and can thus be useful to e.g. evaluate field measurements and model the late stage of the wetting process. The equations are mainly based on results from tests with increasing degrees of saturation under constant void ratio but are also suggested for use with increasing void ratio.

Thermal expansion has been simulated under water-saturated conditions in laboratory tests, which show that expected stress increases occur, followed by falling stresses due to drainage of water. A numerical modelling of the process /Börgesson 1992/ shows that the maximum pore pressure increase amounts to 8 MPa due to the fact that the rock drains the buffer. However, this calculation assumes that the rock acts as a filter for the pore water meaning that the pore water is allowed to enter the rock matrix freely.

Additional experiments need to be done to improve the understanding of the volume change behaviour of initially unsaturated buffer and to better model its evolution.

Time perspective

The water saturation phase is expected to take between 10 and 100 years, depending on the properties of the rock. During this time span, the portion of the expansion that is limited by the consolidation rate (which is controlled by the hydraulic conductivity) probably also takes place. The subsequent volume creep can proceed for thousands of years, but is not judged to be of such a magnitude that it appreciably influences buffer performance. The deviatoric creep will also continue during the lifetime of the repository and its main effect will be the canister sinking (see above) but will also influence the homogenisation of the buffer. As mentioned earlier the friction in the bentonite is counteracting the homogenisation and is responsible for e.g. the following effects:

1. The decrease in buffer density at the buffer/backfill interface is not spread to the entire buffer
2. The penetration of bentonite into the fractures in the rock is limited to about 25 times the fracture aperture
3. There will be a remaining radial difference in density originating from the swelling of the blocks and if present, compression of the pellets

The deviatoric creep can be regarded as a decrease in friction with time. This process, which has been investigated in relation to the canister sinking, is very slow and not expected to have a dramatic influence on the buffer in the lifetime of a repository.

Thermal expansion: Temperature calculations /Thunvik and Braester 1991/ show that the maximum temperature in the bentonite at the canister wall is reached after about 10 years, at the rock wall after about 30 years and furthest away from the canister after another ten years or so. In the most favourable case, water saturation can be reached between the canister and the rock in a few years and in the whole buffer after 10–15 years. In other words, there is a risk that a pressure increase will arise in the interval between 10 and 50 years after deposition. However, the temperature increase is very moderate and slow during this time interval. Furthermore, a temperature decrease takes place simultaneously nearest the canister after about 10 years, which counteracts the effect. As stated above the judgement is that this process is not a problem.

Natural analogues/observations in nature

No natural analogues concerning mechanical behaviour have so far been studied. The existence of relevant natural analogues is probably very limited and difficult to evaluate.

Handling in the safety assessment SR-Can

The process is relevant in all timescales, is influenced by a range of boundary conditions/effects and coupled to a number of other processes.

Early effects

The initial swelling is modelled as part of the integrated initial THM evolution of the buffer, see further Section 2.3.1. Also thermal expansion and interaction buffer/backfill is included in this modelling.

The near-field evolution model /Hedin 2004/ will be used to study the swelling of the buffer and the compaction of the backfill at the end of the saturation phase for different assumptions regarding critical input data like friction and groundwater salinity, see further Section 2.3.1.

Long-term effects

Long-term effects of ion exchange and saline groundwater will be evaluated using empirical relationships described above. The effects of salinity will also be modelled by the Donnan model referred to in Section 2.5.8. This is implemented in the near-field evolution model.

Effects of canister corrosion products: Estimates of volumes and thus of the increase in swelling pressure etc, will be carried out as part of an assessment of integrated, long-term mechanical effects. This will include a quantitative treatment of copper corrosion.

Canister sinking: The process is provisionally neglected, based on the above modelling results. A more developed basis for this assumption, based on a buffer density criterion to justify neglecting of the phenomenon might need to be established. The consequences of canister sinking will be assessed in a residual scenario.

Effects of convergence of deposition hole: These effects will be estimated based on results from ongoing studies as part of discussion of integrated, long-term mechanical effects.

Effects of intrusion into fractures and subsequent colloid formation and dispersion: Neglected as long as the concentration of divalent cations in the groundwater exceeds 1 mM, otherwise the process has to be quantified. See further Section 2.5.10.

Failed canister: Effects of gas generation and of penetration of clay into the canister must be considered in the integrated treatment of a failed canister in relevant scenarios.

Earthquakes: The mechanical effects of earthquakes on the buffer will be handled in separate, integrated assessments in the SR-Can main report, encompassing also earthquakes that do not cause canister failure. Generally, it is noted that a shear movement does not alter the volume of a deposition hole significantly.

Uncertainties

Uncertainties in mechanistic understanding

After complete water-saturation, the swelling process is deemed to be sufficiently well-known and the final density distribution in the buffer can be calculated with sufficient accuracy.

In the long term, swelling properties can change due to transformations and cementation, see Section 2.5.9 “Montmorillonite transformation”. The mechanical consequences of transformations can be assumed to lead a higher hydraulic conductivity and a decrease in swelling pressure.

Cementation effects may cause significant changes in the physical properties of the buffer, since they can produce a material that is brittle and without swelling capacity and thus can crack and open channels and gaps in the buffer. Since this is a chemical process it is treated elsewhere, see Sections 2.5.9 and 2.5.6.

The swelling pressure process and the swelling/compression properties at water saturation are rather well known and can be modelled with sufficient accuracy /Börgesson et al. 1995/.

The mechanical function of water-unsaturated bentonite is complicated to model, and the models that exist today are incomplete, especially for modelling of volume change and swelling pressure. Work is ongoing. The mechanical processes before water saturation are not considered important for safety, but have been investigated in order to improve the general understanding of the saturation phase.

The mechanisms of the different interactions (mechanical interaction buffer/backfill, buffer/rock and buffer/canister) are rather well known regarding the final state after saturation and stress equilibrium.

Thermal expansion: The process is well understood for water-saturated bentonite. For water-unsaturated bentonite the thermo-mechanical theory formation is not complete, but the consequences of this process are deemed in this case to be unimportant for safety.

The largest uncertainty beside the behaviour at unsaturated state concerns the creep. Although a creep model exists and has been verified (for deviatoric stress) the validity for long-term effects is difficult to prove.

Model simplification uncertainties for the above handling in SR-Can

See the above heading.

Input data and data uncertainties for the above handling in SR-Can

Water saturated state: Some uncertainty arises in calculating the size of the swelling pressure after swelling, where the possible deviation is judged to be ± 30 percent, depending on the scatter in swelling pressure measurements and the uncertainty in certain material parameters. Some validation has been done by means of laboratory /Pusch and Adey 1986/ and field tests /Börgesson 1993a/, and continued validation is taking place via the field tests in the Äspö HRL and laboratory tests performed and reported recently /Börgesson et al. 1995, Karnland et al. 2002/ and ongoing tests. Other parameters required are rather well known, e.g. the friction angle (which is a function of density) and the compressibility, which have an uncertainty of 10–20%.

Unsaturated state: Since the mechanical processes during the unsaturated state are rather poorly known, the uncertainties are large. These processes are deemed to mainly influence the path the system will take to reach the saturated state and only to an insignificant degree influence the final, saturated state.

2.4.2 Liquefaction

Overview/general description

Liquefaction is a process implying that a stiff material (soil) turns into liquid due to an affect with short duration, see e.g. /Lambe and Whitman 1969/. It may take place in a loose sand when the pore water pressure is increased either due to a vibration that makes the sand particles float in the pore water (since they tend to go into a higher degree of compaction, but the water temporarily prevents it) or due to a strong upward water flow that releases the effective stresses between the particles (quicksand). It may also take place in clay that has been settled in salty water (forming an open structure with a high water ratio). If the salt is partly washed out by fresh water, the clay structure cannot hold the high amount of water at moulding or vibrations, meaning that the structure collapses when exposed to vibrations.

These two types of liquefaction cannot take place in a bentonite with high density, since the effective stress that holds the clay together is high due to the swelling pressure. This conclusion is also made by /Pusch 2000/. However, a similar phenomenon has been observed during compaction of bentonite blocks at very high water ratios. If the bentonite is compacted at a very high stress to a state where the bentonite is completely water saturated, all further increase in stress will be taken by the water and the bentonite will behave like a liquid. This phenomenon has been observed during uniaxial compaction when liquid bentonite has squirted from the mould.

The process requires a very strong impact of pressure and is rather unlikely to occur in a deposition hole. It can probably only occur at an earthquake and requires a reduced volume of the deposition hole due to an increase in rock stress. A combination of factors may lead to an increase in rock stress of about 15 MPa /Bäckblom et al. 2004/. Estimation according to Kirsch /Brady and Brown 1994/ of the convergence of a deposition hole at such an increase in rock stress may yield a convergence of the hole of about 1 mm.

Table 2-10 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Boundary conditions

The process requires that the rock boundary of the deposition hole be exposed to a sudden pressure increase with associated reduction in the volume of the deposition hole.

Model studies/experimental studies

Block compaction tests have shown that the process may occur. Some laboratory tests are running in order to shed further light on the process. The process will, similarly to the rock shear case, be subjected to an investigation of the worst possible rock response that can result from an earthquake and then followed by investigations of the influence of such a scenario on the buffer.

However, using traditional soil mechanical considerations it can easily be shown that a convergence cannot cause liquefaction. A simple 1-element calculation illustrates the situation.

Table 2-10. Process/variable table for the process Liquefaction.

Variable	Does this variable influence the process?		Does the process influence this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Buffer geometry	Yes	The process will not occur	Yes	The process will not occur
Pore geometry	Yes	“	Yes	“
Radiation intensity	No	“	No	“
Temperature	No	“	No	“
Water content	Yes	“	No	“
Gas content	Yes	“	No	“
Hydrovariables (pressure and flows)	Yes	“	Yes	“
Stress state	Yes	“	Yes	“
Bentonite composition	No	“	No	“
Montmorillonite composition	No	“	No	“
Pore water composition	No	“	No	“
Structural and stray materials	No	“	No	“

A porous soil with the following properties is considered:

- Void ratio e=0.8
- Degree of water saturation S_r=100%
- Initial effective stress (swelling pressure): p=7 MPa
- Initial pore water pressure u=0

The compression properties of the soil skeleton is regulated by the porous elastic function /Börgesson et al. 1995/ and the properties identical to the ones used for modelling water saturated buffer material MX-80.

The *Porous Elastic Model* implies a logarithmic relation between the void ratio e and the average effective stress p according to Equation 2-12.

$$\Delta e = \kappa \Delta \ln p \qquad (2\text{-}12)$$

where κ = porous bulk modulus. Poisson's ratio ν is also required.

κ = 0.2

ν = 0.4

The compressibility of water and solids are

$B_w = 2.1 \cdot 10^6$ kPa (bulk modulus of water)

$B_s = 2.1 \cdot 10^8$ kPa (bulk modulus of solids)

If such a soil is compressed the result will be a compression of the structure, the water and the solids and the resulting total pressure, pore water pressure and effective stress will develop according the relationships provided in Figure 2-11. The calculation was done with ABAQUS.

Figure 2-11 shows that compression of a water-saturated buffer as expected yields an increase in effective stress, due to the compression of the clay skeleton during compression of the water in the pores. An increase in total pressure of from 7 MPa to 150 MPa yields an increase in effective stress from 7 MPa to 9 MPa.

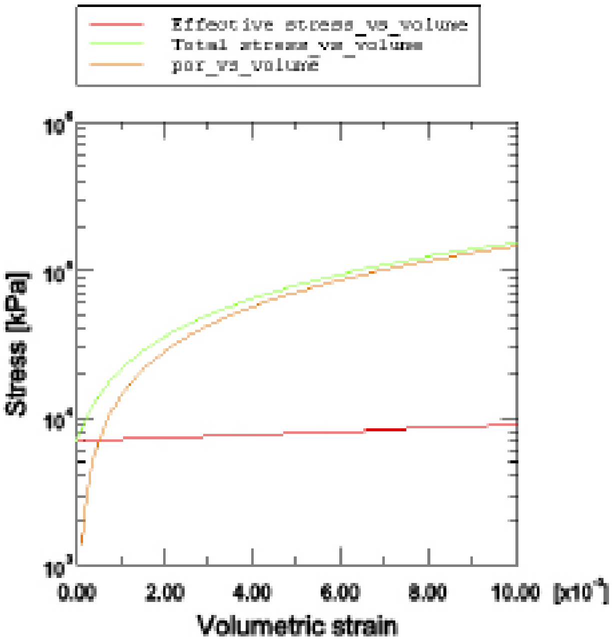

Figure 2-11. *Results of modelling compression of water saturated buffer.*

The mechanisms that induce the type of liquefaction observed during block compaction must thus have another origin than the effective stress theory. An explanation could be that the clay particles (which for montmorillonite really are very thin flakes) are not in direct contact but are separated by water molecule layers. Since these layers at full water saturation are in equilibrium with the external pressure, which is equal to the swelling pressure plus the water pressure, an increase in external pressure will disturb the equilibrium and may change the structure and stiffness of the water so that it becomes liquid if the pressure increase is high and fast enough.

The magnitude of the required pressure increase is not known, but must be investigated in the laboratory. A convergence of the deposition hole of 1 mm will cause a volumetric strain of $1.1 \cdot 10^{-3}$, which according to Figure 2-11 yields a change in total stress in the buffer of about 15 MPa.

Another possible scenario that may occur is an increase in the water pressure in fractures connected to the water-saturated buffer, which may occur at an ice age. This effect has been investigated both by a similar ABAQUS calculation and by tests in the laboratory. Figure 2-12 shows the results of the calculation. An increase in total stress to 200 MPa yields an insignificant decrease in effective stress with 55 kPa (which is caused by compression of the particles).

The effect of high water pressure has been investigated with the following laboratory test:

A bentonite sample of MX-80 with the void ratio $e \sim 0.9$ was confined in a swelling pressure oedometer and the vertical and horizontal total pressure measured. The sample was water saturated through filter stones applied at both ends of the sample. The pore water pressure was regulated by a GDS apparatus connected to the filter stones. The water pressure was then changed and the influence on the total pressure measured. Figure 2-13 shows the results of the tests. The original swelling pressure (effective stress) at no pore water pressure is about 3.4 MPa. At the stepwise increase in pore water pressure to 12 MPa the effective stress (calculated as the difference between the total stress and the pore water pressure) is reduced to about 2 MPa. The effect is thus much higher than expected from the effective stress theory. One reason could be strain in the apparatus that may decrease measured pressure due to increase in void ratio. Estimation of the volume change of the apparatus shows that a change in total pressure of 12 MPa may result in a volumetric strain of about 0.1%, which corresponds to an increase in void ratio from 0.9 to 0.9005. This is far too small to explain the observed drop in effective stress.

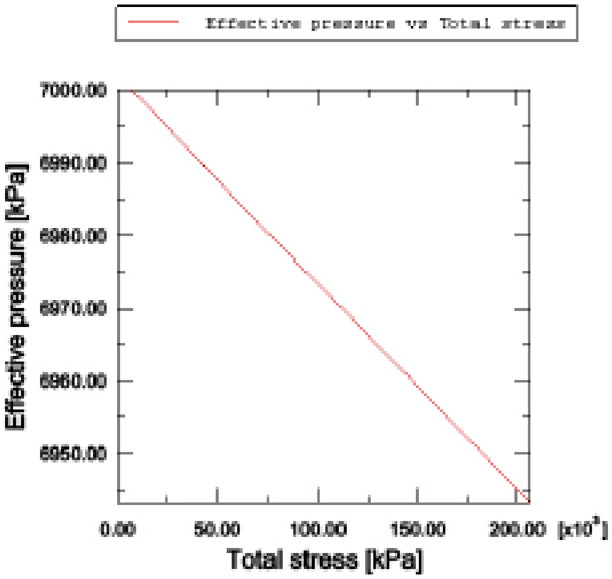

Figure 2-12. *Swelling pressure as a function of applied total stress during pore water pressure increase of 0–200 MPa.*

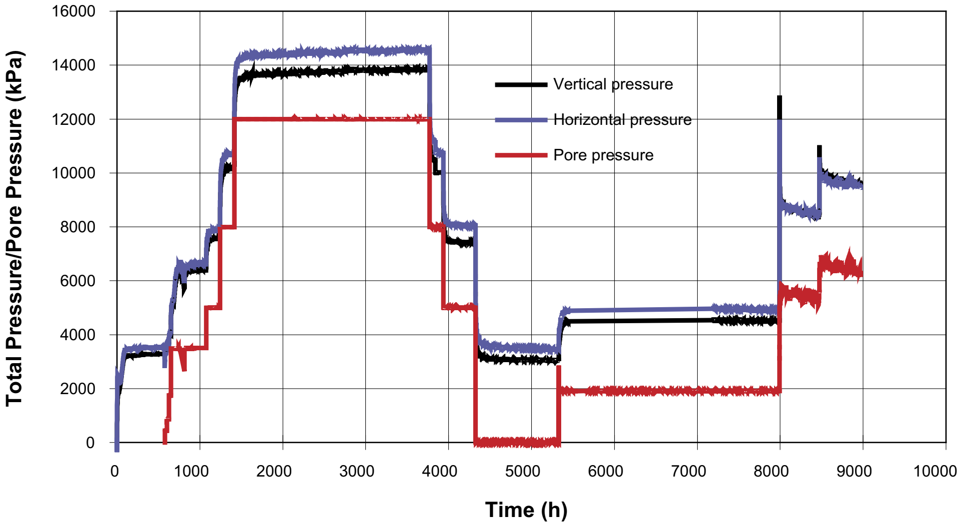

Figure 2-13. *Results of the tests under constant volume in the swelling pressure oedometer. The total pressure is measured during stepwise changes in water pressure.*

Another explanation may be that the effective stress theory is not valid for this material. It has earlier been shown to be valid well enough for normal applications, but perhaps not at the extreme conditions that prevail during processes that may lead to liquefaction. The effective stress theory states

$$\sigma = \sigma' + Au \qquad (2\text{-}13)$$

where

σ = total stress

σ' = effektive stress

u = pore water pressure

A=1.0

If A differs from 1.0 the effective stress theory is not completely valid. The results in Figure 2-13 may be evaluated for each load step as shown in Figure 2-13. The relation between total stress and water pressure can then be written according to Equation 2-13 with

σ' = 3,345 (effective stress (swelling pressure) at u=0)

A=0.90

yielding Equation 2-14

$$\sigma = 3{,}345 + 0.9u \qquad (2\text{-}14)$$

which thus corresponds to the blue line in Figure 2-14. The pink line represents Equation 2-15

$$\sigma - u = 3{,}345 - 0.1u \qquad (2\text{-}15)$$

The "apparent effective stress" according to Equation 4 thus intersects the x-axis (representing no effective stress) at the pore water pressure

u = 33,450 kPa

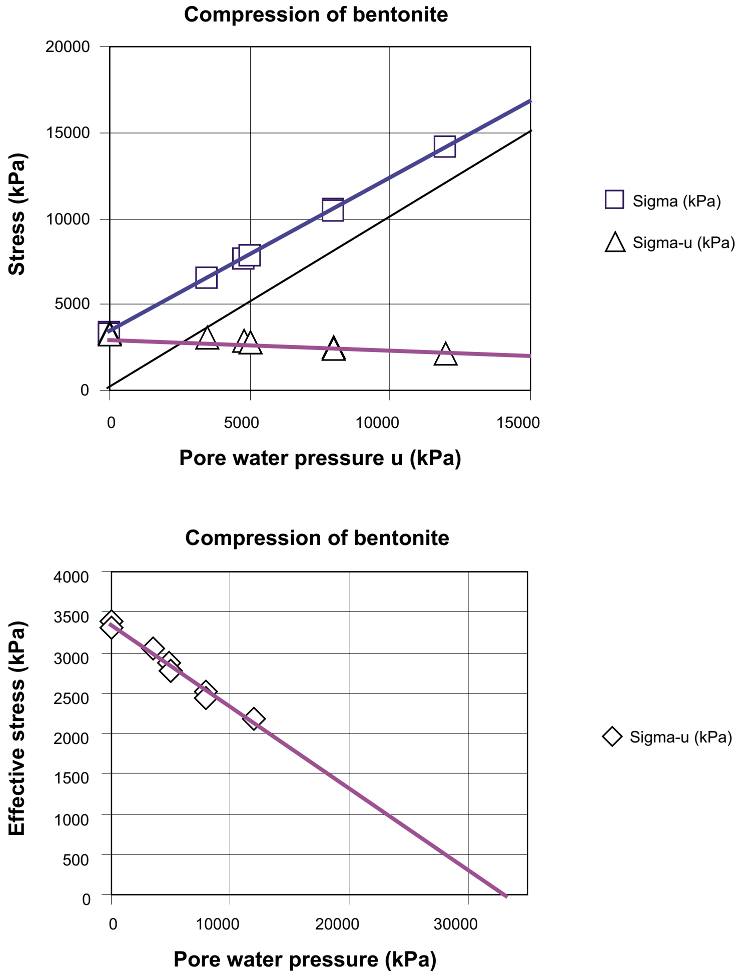

Figure 2-14. *The measurements shown in Figure 2-13 plotted as function of the applied pore water pressure u.*

According to this reasoning a buffer with the void ratio e=0.9 would have no effective stress and thus no strength at the pore water pressure 33,450 kPa, which according to Equation 2-14 corresponds to a total stress 33,450 kPa or 33.5 MPa. If Equation 2-14 is generalized it would imply Equations (2-16) and (2-17).

$$\sigma = \sigma_s(e) + \mathrm{A}u \qquad (2\text{-}16)$$

$$\sigma - u = \sigma_s(e) - (1 - \mathrm{A})u \qquad (2\text{-}17)$$

where

$\sigma_s(e)$ = swelling pressure at the void ratio e

For the average void ratio expected in a deposition hole (e=0.8) the swelling pressure is about 7 MPa, which yields (if A=0.9)

$\sigma - u = 7{,}000 - 0.1u = 0$ at

$u = \sigma = 70{,}000$ kPa

It would thus require a pore water pressure of about 70 MPa in order to yield liquefaction, which is higher than expected as the result of an ice age (20–40 MPa).

If the relation is valid also during compression and subsequent increase in total stress the required total stress to yield liquefaction in half an order of magnitude higher than the expected increase in rock stress (15 MPa). In addition the required compression of the buffer for yielding such a high stress is a volumetric strain of about 0.4% according to the calculation shown in Figure 2-11 which corresponds to a convergence of the deposition hole of about 3.5 mm. This is clearly higher than expected (1 mm).

Natural analogues/observations in nature

Not applicable.

Time perspective

The process may occur anytime during the lifetime of the repository. The process requires both completion of the saturation process and an earthquake.

Handling in the safety assessment SR-Can

If the reasoning and theories stated above are correct it would mean that liquefaction may occur either due to a very high water pressure or a convergence of the deposition hole resulting in a very high water pressure. However the required water pressure is higher than could be expected under any currently recognized scenario and the expected maximal stress increase in the rock and convergence of the deposition hole are clearly lower than required for liquefaction to appear.

The process is therefore not considered within the SR-Can study

Uncertainties

There are several weaknesses and questions related to the current level of knowledge on the liquefaction issue:

- Only one test has been performed
- The results are strongly extrapolated in order to reach liquefaction
- The parameter A is determined for a too low swelling pressure
- The tests entailed pore pressure increase and it is not certain that the same observation and theory is valid when the stresses are reached by increasing the total stress
- Although Equation 2-17 may be valid it has not been shown that pore pressure equal the total stress yields liquefaction

A number of additional tests should thus be performed in order to further study the validity of the presented theories. The following 3 tests are primarily desired:

- Repetition of the test with pore water pressure increase at constant total volume with a bentonite that has a lower density in order to be able to reach liquefaction at u=12 000 kPa using the available equipment
- Repetition of the test with pore water pressure increase at constant total volume to higher pore water pressure and at higher bentonite density
- Tests with increased total stress and measurement of pore water pressure until liquefaction can be observed.

2.5 Chemical processes

2.5.1 Introduction

Bentonite minerals

High quality commercial bentonites normally contain over 80% of montmorillonite, which gives different bentonite products similar properties in many respects. The distribution of accessory minerals may vary within, and especially between different quarries. Typical accessory minerals are feldspars, quartz, cristobalite, gypsum, calcite and pyrite.

The montmorillonite mineral belongs to the smectite group, in which all the minerals have an articulated layer structure. The thickness of an individual mineral layer is around 1 nm (Figure 2-15) and the extension in the two other directions is often several hundred nanometers. Each layer is composed of a central sheet of octahedrally coordinated cations, which on both sides is linked through shared oxygens to sheets of tetrahedrally coordinated cations. Clay minerals of this type are often referred to as a 2:1 layer structures.

By definition of the montmorillonite mineral, the following applies. The octahedral sheet has aluminum as central ion, which is partly substituted principally by Mg. The tetrahedral sheet has silicon as central ion, which partly may be substituted principally by aluminum. The substitutions results in a net negative charge of the montmorillonite layer in the range of 0.4 to 1.2 unit charges per $O_{20}(OH)_4$-unit, and the octahedral charge is larger than the tetrahedral. The induced negative layer charge is balanced by cations (c) located between the individual layers (interlayer space). A variable number (n) of water molecules may be intercalated between the individual mineral layers.

The montmorillonite ideal formula may consequently be written:

$Si_{8-x}Al_x$ $Al_{4-y}Mg_y(Fe)$ $O_{20}(OH)_4$ $c_{x+y}n(H_2O)$ $(x < y)$ and
tetrahedral octahedral interlayer $0.4 < x+y > 1.2$

and the structure may schematically be illustrated as in Figure 2-15.

Bentonite pore-water

Ions in a water solution reduce the water chemical potential, and a concentration difference between solutions normally leads to water transport from the high potential (low concentration) to the low potential volume. In parallel, ions will diffuse from the high concentration to low concentration volume, and the equilibrium condition, i.e. equal chemical potentials, leads to uniform ion concentration.

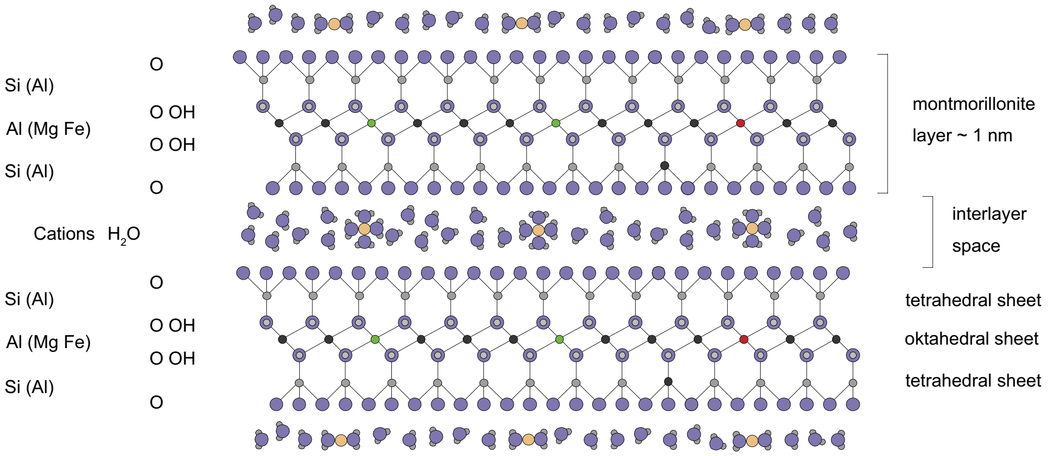

Figure 2-15. *Edge view cartoon of two montmorillonite layers with interlayer cations and water molecules.*

The total suction of a soil, as described in Section 2.4.1, includes osmotic suction and matric suction. By definition, the osmotic suction is due to lowering of the chemical potential in pore-water by ions, and the matric suction refers to the lowering of the chemical potential of the pore-water by mineral surface interaction.

In bentonite, the conditions are extraordinary due to the negatively charged montmorillonite layers and the charge compensating cations in the interlayer space. Water molecules can be intercalated between the individual montmorillonite layers to create an interlayer ionic solution. The cations cannot freely diffuse away from the mineral surface because of the demand for electrical neutrality. Water will consequently be transported into the inter-layer space, if water with a higher chemical potential is available, and the interlayer distance will increase, which is synonymous with bentonite swelling. This water uptake will continue until the chemical potentials equal, which in the case of a pure water source theoretically leads to infinite swelling. The extent of water uptake in bentonite may thereby be orders of magnitude larger and have a different character than in other soil materials.

In a fixed total volume, the water uptake into the interlayer space will reduce the volume of initially larger pores. The uptake is forced to stop when the total available pore volume is completely filled with introduced water. At this full water saturation, water will continue to move in order to level the interlayer ion concentration and thereby the chemical potential in the system. The interlayer distances will thereby increase in interlayer space with high concentration on the expense of interlayer space with low concentration, and the final distances will be a function of the local montmorillonite layer charge. The remaining difference in ion concentration, between the high concentration interlayer solution and the water supplying solution, leads to an osmotic pressure build-up in the clay (swelling pressure), which equals the chemical potential of water in the system. The homogenization of the pore size, due to the leveling of the chemical potential, may be partly counteracted by mechanically stable structures, e.g. in volumes with complicated stacking of the montmorillonite layers, or in clusters of accessory minerals. In extreme cases the pore-water in such clusters may eventually be in equilibrium with the water supplying solution, without influence from the surrounding montmorillonite charge compensating cations.

The degree of final pore size homogeneity has been analyzed and extensively discussed in the literature, and quite different conceptual and quantitative models have been proposed. The conditions are of major importance since the pore-size distribution governs the possible transport of colloids (2.5.4).

The concentration of the charge compensating cations in the interlayer space is highest close to the negatively charged montmorillonite surfaces and will decrease drastically with distance from the surfaces. The distribution, which may ideally be calculated by use of the Poisson-Boltzmann equation, is of major importance for the ion equilibrium with other ions in the system, which may origin from an external solution (2.5.8) or from accessory minerals in the buffer (2.5.6).

The volume of a deposition hole and the corresponding buffer mass are predetermined, and the interlayer cation concentration can consequently be calculated. The total pore volume in the buffer in one deposition hole is around 5,250 liters, and the bentonite mass is around 19,250 kg. The montmorillonite layer charge may be experimentally determined and are usually given as cation exchange capacity (CEC). The reference bentonites have a CEC of around 0.75 equivalents per kilogram clay material, which give a total cation content of around 14,430 equivalents in each borehole. The mean cation concentration in this system is consequently almost 3 M for monovalent ions if it is in equilibrium with pure water. Figure 2-16 shows the cation distribution in the interlayer for three different interlayer distances at equilibrium with pure water, as calculated by Poisson-Boltzmann equation.

Cementation

The term “cementation” has often been used in a broad sense to describe effects of chemical and mineralogical processes which can lead to various changes in the rheological properties of the buffer material, for example increased mechanical strength, brittleness or reduced swelling capacity. A number of completely different processes could conceivably cause similar effects,

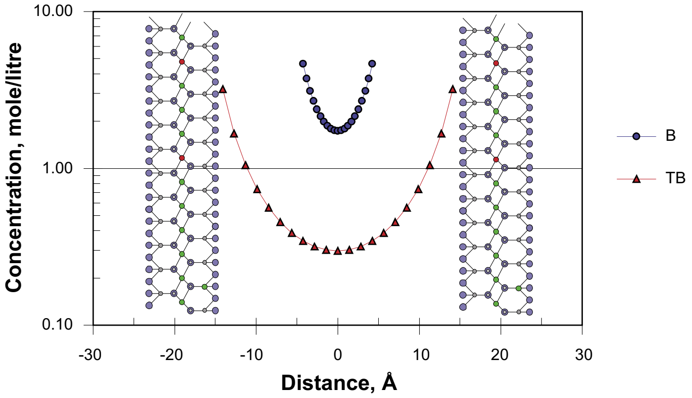

Figure 2-16. *Concentration distribution of charge compensating cations for two different interlayer spacings. B represents mean buffer spacing of around 1 nm, TB represents the mean interlayer spacing in the tunnel backfill material of around 3 nm, and R represents a randomly chosen 10 nm spacing. Two scaled montmorillonite mineral layers are shown to illustrate the geometry for the R-case.*

and the underlying reactions can occur in the molcular structure of the montmorillonite mineral layer, in the interlayer space, or in accessory minerals. The resulting cementation does not necessarily have to appear in the same area as the underlying process, since released species can be transported in the buffer by different prevailing gradients (thermal, concentration, etc) and be precipitated in various locations and forms. The chemical processes discussed for the buffer/backfill include those reactions that have been offered as possible causes of cementation of the buffer. Cementation will, however, not be discussed as a process in its own in this context.

2.5.2 Advective transport of species

Overview/general description

Solutes (dissolved substances) and colloids can be transported with pore water by pressure-induced flow: advection. In this manner, solutes move from areas of higher water pressure to areas of lower pressure. The process leads to redistribution of solutes in the pore water and thus affects the pore water composition. There are several possible causes of pressure gradients in the buffer material, e.g. external water pressure, temperature induced volume change of the water, ion concentration gradients in water, and affinity for water in the bentonite. The advective transport of materia is a direct function of water flow in the buffer, which is comprehensively described in Section 2.3.

Advection is of importance in the buffer during the unsaturated period when a net flow of water takes place in the buffer. The principal flow during this phase takes place in the direction towards the canister, provided that the rock supplies the buffer with groundwater. After placement of a canister, a minor flow will initially also take place in the direction from the canister due to the transient temperature gradient.

Under saturated conditions, the transport of solutes in the pore water is expected to be dominated by diffusion, see Section 2.3.2. Exceptions may be sudden events such as gas pulses or earthquakes, which can cause local pressure changes in the buffer. The improbable condition with a failure at the bottom of a canister may lead to a partly water-filled canister and hydrogen gas pressure acting on the water. The gas pressure may build up to reach at least the bentonite swelling pressure, which would lead to a significant advective water flow from the canister.

Table 2-11 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Table 2-11. Process/variable table for the process Advective transport of species.

Variable	Does this variable influence the process? Influence present?	Handling of influence?	Does the process influence this variable? Influence present?	Handling of influence?
Buffer geometry	Yes	Buffer dimensions are included in calculations	No	
Pore geometry	Yes	Defines the hydraulic conductivity	(Yes)	See 2.3.1
Radiation intensity	No		No	
Temperature	Through viscosity	Effect is small and not considered in transport calculations	(Minor)	
Water content	(Yes)	See See 2.3.1	No	
Gas content	Reduced flow in unsaturated clay	Advective transport of species during the unsaturated stage is not and issue	(Transport of dissolved gas)	Advective transport of dissolved gas is not an issue
Hydrovariables (pressure and flows)	Yes	Hydraulic conductivity is used to determine whether advection can occur	Yes	Determines the advective flow
Stress state	(Yes)	Swelling pressure is used to determine whether advection can occur	(Yes)	Through pore geometry
Bentonite composition	No		No	
Montmorillonite composition	No		No	
Pore water composition	Yes	Determines the hydraulic conductivity	Yes	Determines the exchange of species
Structural and stray materials	(Alternative transport paths)	Not considered in SR-Can – no route to alternative path has been found	No	

Boundary conditions

The external boundary condition for this process is the hydraulic gradient across the buffer.

Model studies/experimental studies

Several studies by SKB and others have examined water flow in bentonite material, both during water uptake and after complete water saturation, and a wealth of quantitative data, which describes water transport, is available on different physico-chemical conditions, e.g. densities, temperatures, salt solutions (see Section 2.3.2).

The Long Term Tests of Buffer material (Lot) field test at Äspö HRL shows an increase in total ion concentration in the porewater compared to what is originally present in the bentonite as a consequence of the salinity of the saturating groundwater /Karnland et al. 2000/. Precipitation of calcite and gypsum close to the central heater indicate ion enrichment (Section 2.5.6).

Natural analogues/observations in nature

Comment: Sediments rich in smectite may keep large chemical gradients over geological timescales /Neuzil 2000/.

Time perspective

Advective flow transport in conjunction with water saturation takes place on a timescale of up to hundreds of years. Flow transport after water saturation is expected to be negligible in relation to diffusive transport.

Handling in the safety assessment SR-Can

Before saturation: No detailed modelling of advection is required. It should be noted that the composition of the porewater will be influenced by the composition of the intruding water during saturation. The groundwater composition should be considered when defining initial conditions for modelling of the chemical evolution after saturation, see further Section 2.5.6.

After saturation: Based on the scenario specific evaluation of water transport under saturated conditions, process 2.3.2, advection will normally be neglected compared to diffusion. If the expected low hydraulic conductivity is for some reason not maintained, advection will be included in the modelling of the canister corrosion and of radionuclide transport.

Handling of variables influencing this process: See process 2.3.2

Failed canister: Advective flow from the canister due to hydrogen gas pressure will be calculated as a special case in the radionuclide transport calculations.

Earthquakes: Pressure transients may arise, but will not be prevailing over the buffer over timescales that could lead to significant water flow.

Uncertainties

Uncertainties in mechanistic understanding

See Section 2.3.2 for uncertainties concerning water advective transport.

Model simplification uncertainties for the above handling in SR-Can

Unsaturated conditions: see Section 2.3.1.

Saturated conditions: The process can be modelled with a standard mass-transfer approach. The main uncertainty lies in the coupling between the fractured rock and the porous buffer.

Input data and data uncertainties for the above handling in SR-Can

Unsaturated conditions: See Section 2.3.1.

2.5.3 Diffusive transport of species

Overview/general description

Solutes can be transported in stagnant pore water by diffusion, following concentration gradients. Solutes thereby move from areas of higher concentration to areas of lower concentration. The process leads to a redistribution of dissolved porewater constituents as well as radionuclides in the porewater. Therefore, diffusion is a critical process for radionuclide migration in the buffer, but also affects the actual porewater composition.

The diffusion process is strongly coupled to nearly all chemical processes in the buffer, since it accounts for transport of reactants to and reaction products from the processes. Diffusion of Na^+ and Ca^{2+} ions is, for example, of crucial importance to ion exchange processes, diffusion of K^+ is an important limiting factor for the illitization process, etc. Diffusion is thereby a central process for the entire chemical evolution in the buffer.

Diffusion in bentonite has been thoroughly studied in conjunction with radionuclide transport. Diffusion equations for radionuclides (as well as some experimental measurement techniques relevant for determining the respective parameters) are described in detail in /Yu and Neretnieks 1997/.

Diffusion in a porous medium takes place according to Fick's first law (Equation 2-18):

$$J = -D_p \varepsilon \, dC_p/dx \qquad (2\text{-}18)$$

Where: J is the diffusive flux, D_p the diffusion coefficient in the pore solution, ε is the porosity and C_p the concentration of the diffusing species.

The pore diffusion coefficient in a solution-filled pore is lower than the diffusion coefficient in an unconfined volume of the same solution, D_w. This is mainly due to the tortuosity of the pores, which increases the length of the diffusion path. The relationship between D_p and D_w is:

$$D_p = D_w \, \delta/\tau^2 \qquad (2\text{-}19)$$

Where: δ is the physical constrictivity and τ the tortuosity of the pores. The constrictivity takes into account any narrowing or widening of pores along the flow path. Since bentonite is viewed as a homogeneous porous medium on a macroscopic level, δ is usually set equal to unity.

Fick's second law, taking into account conservation of mass, describes changes in concentration of a diffusing species in time and space. For diffusion of a sorbing species in a porous material, it can be formulated as follows (Equation 2-20):

$$\varepsilon \, \partial C_p/\partial t + \rho \partial q/\partial t = \varepsilon \, D_p \, \partial^2 C_p/\partial x^2 \qquad (2\text{-}20)$$

where ρ is the material's bulk density. For conditions where sorption is linear, Equation (2-21) can be written:

$$\partial C_p/\partial t = D_e/(\varepsilon + K_d \, \rho) \, \partial^2 C_p/\partial x^2 = D_a \, \partial^2 C_p/\partial x^2 \qquad (2\text{-}21)$$

where K_d is the distribution coefficient (see Section 2.5.5), D_e is the is the effective and D_a the apparent diffusion constant, which are defined as follows:

$$D_e = \varepsilon D_p + K_d \rho \, D_s \qquad (2\text{-}22)$$

$$D_a = D_e/(\varepsilon + K_d \rho) \qquad (2\text{-}23)$$

When sorbing solutes are present at trace levels, sorption is independent of their concentration (i.e. where the concept of a linear sorption isotherm applies), C_p can be replaced by the total concentration in the porous material by multiplying by $\varepsilon + K_d\rho$ (the capacity factor, α) in Equation (2-23), which gives:

$$\partial C/\partial t = D_a \, \partial^2 C/\partial x^2 \qquad (2\text{-}24)$$

where C is the total concentration. Equation (2-24) is the relation that is normally used for diffusion studies of radionuclides in bentonite. For diffusion of inert, non-interacting species, D_a is equal to D_e/ε (since anions interact with the negative charge of clay surfaces, i.e. are not inert in this sense, this relation does not apply directly to anions; this relation holds, however, if the physical porosity ε is replaced with a reduced value for anion-accessible porosity, ε_{anion}).

Enhanced apparent cation diffusion: It has been observed in several cases that the apparent diffusion coefficient (D_a) for cations and their respective distribution coefficient (K_d) have not agreed. D_a has been higher than expected from K_d and traditional porewater diffusion-sorption theory. While several explanations of this phenomenon have been proposed (see below), it is of foremost importance to recognise that an agreement of D_a and K_d is only to be expected for self-consistent datasets. I.e. both D_a and K_d need to correspond to the same set of conditions, in particular to the same porewater composition. Thus, several of the discrepancies between

D_a and K_d observed in the past can be traced to the fact that incompatible conditions have been compared. In particular, D_a values that invariably correspond to the pore water composition in compacted bentonite have been compared directly with K_d values from batch experiments involving typically much more dilute solutions. Given that K_d values are derived for relevant porewater conditions, sorption and apparent diffusion coefficients for many elements agree within the overall data uncertainty /Ochs et al. 2003, Bradbury and Baeyens 2003/.

Nevertheless, there are cases where it seems clear that certain cations may have enhanced diffusivities, which must be taken into consideration in safety assessments. The presently available information suggests that these cases are largely restricted to relatively mobile and cationic elements: Cs, and sometimes Sr and Ra /Ochs et al. 2003/.

Enhanced apparent cation diffusion can be explained by a cation excess in the diffuse layer (the outer portion of the electrical double layer, EDL) extending from negatively charged clay surfaces into the pore space /Kato et al. 1995, Sato et al. 1995, Ochs et al. 2001/, see also Section 2.5.5. Note that cation excess (as well as anion deficit, see below) have been well established in clay chemistry /see e.g. van Olphen 1991/. Cations thus have an alternative transport pathway where their dissolved concentrations, and therefore the respective concentration gradients, are higher than in the actual pore solution (even though the diffusion coefficient in the diffuse layer could be lower than in the pore solution). Note that this additional pathway is available to cations that are accumulated in the diffuse layer, thereby retaining their mobility parallel to (but not perpendicular to) a mineral surface; it is not available to ions that are specifically (i.e. through chemical inner-sphere bonding) sorbed at surface complexation (or ion exchange) sites.

While presumably based on the same underlying process, the so-called surface diffusion mechanism /Muurinen 1994, Eriksen and Jansson 1996, Yu and Neretnieks 1997/ makes a direct link with actual sorption by introducing an additional surface diffusion coefficient that is multiplied with K_d. As pointed out above, however, there is no reason to assume that specifically sorbed species retain their mobility. A reduction of K_d in highly-compacted bentonite due to a decreased accessibility of surface sites had also been considered as a possible explanation for the disagreement of diffusion data with batch K_d values /Wanner et al. 1996/, but it was shown by /Kato et al. 1995/ that the entire physical porosity in compacted bentonite is accessible.

Anion exclusion: With increasing density, the pore width in compacted bentonite decreases. At high degrees of compaction, the pore width is small enough to cause a superimposition of the electrical double layers between two negatively charged pore walls. At this point, the anion deficit in the diffuse layer pointed out above significantly decreases the available diffusion pathway for anions, giving rise to a phenomenon known as anion exclusion. Evidence from several different studies suggests that the overlap of EDLs occurs at a dry density of about 1,200–1,500 kg/m^3 /Kozaki et al. 1998, Karnland 1997, Ochs et al. 2001/. The effect of anion exclusion becomes less at high salinities, because high ionic strength leads to a depression of the EDL /Stumm and Morgan 1996/. The safety-related importance of anion exclusion is considerable – it is one of the few phenomena that limit the transport of non-sorbing anions from a damaged canister.

Table 2-12 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Influence of pore geometry: The influence of pore geometry is included by the presence of parameters that account for tortuosity and constrictivity in the equations for diffusion coefficients. Typically, the term δ/τ^2 is obtained based on diffusion measurements for HTO.

Influence of temperature: Based on the influence of temperature on the diffusivity of ions in free water /Robinson and Stokes 1959/, it can be expected that D_e will increase about twofold when temperature is increased from ambient conditions to about 50–60°C.

Table 2-12. Process/variable table for the process Diffusive transport of specie.

Variable	Does this variable influence the process?		Does the process influence this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Buffer geometry	Yes	Buffer dimensions are included in calculations	No	
Pore geometry	Yes	Defines the magnitude of the diffusivities	Possibly indirectly through influence on porewater composition and swelling	
Radiation intensity	No		No	
Temperature	Yes	The temperature dependence of the diffusivity is not included in the transport calculations. The importance is regarded as small	No	
Water content	No (saturated conditions assumed)		No	
Gas content	No	(Saturated conditions assumed)	In case of dissolved gases such as CO2 or CH4	Diffusive transport of gases is considered – see also 2.3.3
Hydrovariables (pressure and flows)	Saturated conditions assumed		No	
Stress state	Indirectly through pore geometry		Possibly indirectly through influence on porewater composition and swelling	
Bentonite composition	Through pore water composition	Defines the magnitude of the diffusivities	Indirectly through influence on porewater composition	
Montmorillonite composition	Extent of the EDL depends on magnitude of charge and physical pore width	Defines the magnitude of the diffusivities	Composition of exchangeable ions: indirectly through influence on porewater composition	
Pore water composition	Extent of EDL depends on ionic strength	Defines the magnitude of the diffusivities	Through diffusive transport of main constituents	See 2.5.9
Structural and stray materials	(Through influence on physical pore width)	No stray materials within the buffer are considered	(Possibly indirectly through influence on porewater composition)	

Influnce of bentonite/montmorillonite composition and structural/stray materials: The diffusion properties are dependent on the interlamellar space in the bentonite that is in turn dependent on the permanent charge characteristics and the composition of the exchangeable cations. Soluble stray materials may exert an effect through influencing the porewater composition. Structural and stray materials may also influence pore geometry.

Influence of porewater composition and speciation: Different species of the same element can have radically different diffusivities. This holds for free water diffusivities, but in particular for diffusion in bentonite pores. Due to their interaction with the diffuse layer extending from negative clay surfaces, diffusivities decrease in the order anionic species < neutral species < cationic species. For example, strontium has lower diffusivity at high concentration of sulphate, which can be explained by the formation of the neutral complex $SrSO_4$ /Ochs et al. 2001/. Changes in porewater composition that cause changes in ionic strength influence diffusion also by affecting the extent of the EDL.

Influence of sorption: The influence of sorption is taken into account in the equation for D_a.

Influence of buffer density: The transport of radionuclides in bentonite is influenced by the density of the material (the degree of compaction). This is a direct consequence of the corresponding change in porosity. In addition, the presence of soluble impurities will lead to changes in porewater composition and in particular to an increase of ionic strength as a function of density. The influence of porewater composition is discussed above. In most experiments, the apparent diffusivity decreases with increasing density.

Influence on buffer variables: As pointed out above, the diffusion process is coupled to nearly all chemical processes in the buffer through the diffusive transport of reactants. How chemical processes, such as exchange reactions of major ions, may further influence other buffer variables is discussed in Section 2.5.5.

Boundary conditions

The transfer of species from the bentonite to the rock can be visualised as the diffusion of dissolved species from the bentonite into flowing water in the near-field fracture network (equivalent flow rate or Q_{eq}). The equivalent flow rate can be derived by solving the boundary layer theory equations for diffusive transport into flowing water. The Q_{eq} depends on the geometry of the contact area, the water flux, the flow porosity and the water diffusivity.

Model studies/experimental studies

A large number of investigations are described in the literature concerning diffusion experiments in bentonite and similar clays; see /Yu and Neretnieks 1997/ for a good overview and compilation of diffusion coefficients. Additional results form more recent studies are discussed in the data report /Ochs and Talerico 2004/. Due to experimental reasons, most diffusion studies are performed as transient in-diffusion experiments. These experiments yield D_a, which is a lump-sum representation of all processes relevant for radionuclide migration, including diffusion and sorption. This holds in particular for moderately and strongly sorbing radionuclides. Steady-state through-diffusion studies, which can yield D_e and porosity, are largely restricted to mobile tracers (Cs, HTO, anions).

/Yu and Neretnieks 1997/ also give a detailed discussion of different experimental methods and how the results can be interpreted. For comparisons of data from different studies, it is important to observe which technique has been used and how the diffusivities have been determined. If, for example, metal filters have been used, they can greatly influence the results. It also has to be realised in this respect that the extraction of diffusion coefficients invariably involves fitting of experimental data to the diffusion equations described above.

Few attempts have been made so far to derive diffusion coefficients through semi-mechanistic models. Some examples are discussed above in the context of anion exclusion and enhanced cation diffusion.

Natural analogues/observations in nature

The usefulness of natural analogues for determining diffusion constants is limited due to the difficulty of determining what conditions existed in the past.

Time perspective

Diffusion processes in the buffer material are of the greatest importance on all timescales. If the canister is intact, the process is of importance for the stability of the canister and the buffer. In the case of a defective canister, slow diffusion (which may include sorption, see Equation 2-23) is very important in delaying, reducing and in many cases almost completely preventing releases of radionuclides.

Handling in the safety assessment SR-Can

Before saturation: The process is neglected since advection dominates.

After saturation: The process is included in the scenario specific modelling of the buffer chemical evolution for the thermal phase and the post-thermal long-term phase, see heading "Handling" for process 2.5.6. The process is treated in a simplified way with identical diffusivity for all elements in the buffer chemical evolution.

Failed canister: Included in the modelling of radionuclide transport for the long-term phase, see heading "Handling" for process 2.6.1. For the treatment of radionuclide diffusion, element-specific effective diffusivities are used together with corresponding porosities (see /Ochs and Talerico 2004/ for the definition of data and associated uncertainties).

Boundary conditions: See Sections 2.5.6 and 2.6.1 referred to above.

Handling of variables influencing this process: Dependence on buffer density and bentonite-type, expected ionic charge of diffusing species, ionic strength and temperature is considered in selecting diffusion constants for transport of radionuclides. For the treatment of diffusion within the buffer chemical evolution, see Section 2.5.6.

Handling of variables influenced by the process: The diffusive transport of radionuclides is calculated according to the processes outlined in Section 2.6.1.

Uncertainties

Uncertainties in mechanistic understanding

Because of the experimental inaccessibility of bentonite pores, diffusion data are of macroscopic nature and are not well suited for mechanistic interpretation. On a mechanistic level, the main shortcomings probably lie in the understanding of EDL properties as well as porewater structure and their influence on diffusion (and sorption) processes in compacted bentonite. This is particularly true for high densities that lead to an overlap of opposing EDLs.

The basic processes of enhanced cation diffusion and anion exclusion have been discussed above. The processes giving rise to these phenomena are the establishment of a cation excess and an anion deficit in the diffuse layer extending from a negatively charged mineral surface. Thus, these phenomena are caused by the effects of enhanced or diminished ion concentrations in the volume of the porespace, rather than actual available porosity or different diffusivities. However, several approaches can be used to include the effects of this process in the diffusion Equation (2-23) that is used to define D_a: /Sato et al. 1995, Ochs et al. 2001/ expressed both cation excess and anion deficit through a concentration-correction factor for constrictivity (which leads to a decrease of D_e for anions and increase of D_e for cations), while assuming that the entire physical porosity is available for diffusion. Alternatively, it may be more practical to express this correction factor directly through the diffusion-available porosity, as the anion deficit in the diffuse layer leads to a decrease of the capacity factor α (which includes porosity, but not constrictivity). In clay chemistry, anion exclusion is also expressed by actual negative sorption /van Olphen 1991/, which would also decrease α. Similarly, cation excess and sorption will increase α.

For the selection of radionuclide diffusion data and uncertainties for SR-Can /Ochs and Talerico 2004/, anion exclusion was taken into account through a decrease in D_e and a reduced diffusion-available porosity. Enhanced cation diffusion was accounted for by an increase in D_e in combination with the physical porosity.

Model simplification uncertainties for the above handling in SR-Can

As pointed out above, diffusion is represented in a simplified way, through the use of selected constant effective diffusion coefficients and available porosities in the relevant transport codes (see Sections 2.5.6 and 2.6.1). In that sense, the diffusion input parameters have to be viewed as conditional; i.e. their application will only be valid under the conditions considered in data derivation. Therefore, uncertainties will be related to the selection of consistent conditions. If, for example, the THM processes occurring during buffer evolution will lead to a significant alteration of bentonite properties, it may be necessary to use input parameters that differ form those for standard MX-80 bentonite.

In principle, this situation could be resolved by directly including diffusion processes in the model used for consequence calculations, which would require a THMC model approach. However, in addition to the great difficulties still associated with coupling THM processes on the one and C processes on the other hand, the present state of the art of quantifying radionuclide diffusion in compacted bentonite does not allow this. To date, semi-mechanistic models have been proposed and tested only for a few elements (Cs, Sr, anions; see above). At the same time, formany relevant radionuclides there is a clear lack of systematic data from through-diffusion experiments that would be needed to develop further diffusion models in a meaningful way.

While the abovementioned models are clearly still simplified, they appear to be quite robust as shown by the results of blind model predictions that are consistent with experimental data for several bentonites and over a range of densities /Ochs et al. 2001/. The respective model outputs are also consistent with the selections made for SR-Can. In addition, /Ochs and Talerico 2004/ used the selected D_e values and corresponding K_d values for each element (and relevant oxidation state) to calculate apparent diffusivities, which were then compared to independent experimental data to provide an additional evaluation of the consistency of selected sorption and diffusion parameters. Based on the present evidence, it is expected that the direct use of diffusion parameters will not introduce significant additional uncertainties, given that important boundary conditions in SR-Can will be similar to the conditions considered in the derivation of input data.

Input data and data uncertainties for the above handling in SR-Can

Input data to SR-Can are effective diffusivities and available porosities to be directly used in consequence calculations. Data and uncertainties as a function of bentonite density are given in /Ochs and Talerico 2004/, from which data for consequence calculations are chosen in the SR-Can data report. In comparison to the uncertainties discussed above, the compositional difference between MX-80 and Deponit CA-N bentonite is not expected to have a siginificant influence on radionuclide diffusion. Figure 5-4 in /Ochs and Talerico 2004/ shows that the difference in experimental D_e values obtained on bentonites with smectite contents ranging from about 50% to about 95% is not significant in comparison to the scatter that can be observed for individual studies. In particular, there is no clear trend of D_e as a function of smectite content. Similarly, there is no experimental evidence for an influence of the composition of exchangeable cations on D_e. /Choi and Oscarson 1996/ measured D_e values for iodine as well as for HTO in Ca- and Na-Avonlea bentonite, and their results suggest that the diffusion behaviour of both tracers is the same in both materials.

2.5.4 Colloid transport

Overview/general description

Particles with sizes of the order of 10^{-9} to 10^{-6} m (colloids) could form on dissolution of the fuel. The diffusive transport of fuel colloids through highly-compacted bentonite is, however, assumed to be negligible, due to the tortuosity and small size of the bentonite pores. At emplacement the bentonite has a water ratio of 17% (weight of water divided by weight of solid), which corresponds to a water film with a thickness of $6 \cdot 10^{-10}$ m between the individual montmorillonite flakes (interlayer distance). Larger pores, between the original bentonite grains from which the blocks are produced, make up the remaining pore space. The water film thickness increases during water saturation, and the final theoretical mean interlayer distance is around 10^{-9} m, which obviously would dramatically reduce colloid transport. However, a complete homogenization of the bentonite cannot be expected, and a certain variation in the final pore size will remain also at full saturation. The disjoining force (swelling pressure), and internal friction that counteract the homogenization may be seen as governing variables.

Experiments with 15 nm gold colloids show that the microstructure of a bentonite with a dry density of 1,000 kg/m^3 effectively filters gold colloids /Kurosawa et al. 1997/. This corresponds to a saturated clay density of about 1,640 kg/m^3. However, organic colloids will diffuse through bentonite, but the transport capacity is limited (see below).

Table 2-13 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Table 2-13. Process/variable table for the process Colloid transport.

Variable	Does this variable influence the process?		Does the process influence this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Buffer geometry	No		No	
Pore geometry	Decisive importance	A lowest buffer density to facilitate colloid transport is defined	No	
Radiation intensity	No		No	
Temperature	Very minor	Excluded – No data available	No	
Water content	No (if saturated conditions assumed)		No	
Gas content	No (if saturated conditions assumed)		No	
Hydrovariables (pressure and flows)	No (if saturated conditions assumed)		No	
Stress state	Indirectly through pore geometry		No	
Bentonite composition	No		No	
Montmorillonite composition	Through layer charge	A lowest buffer density to facilitate colloid transport is defined	No	
Pore water composition	Possibly a very minor effect through viscosity	Excluded – No data available	No	
Structural and stray materials	No		No	

Boundary conditions

The process only considers the transport of colloids from the canister interior to the rock contact.

Model studies/experimental studies

/Kurosawa et al. 1997/ reports that 15 nm gold colloids are effectively filtered out at a dry density of 1,000 kg/m^3 for bentonite/sand mixtures with a sand content of up to 40%. At 50% sand there is an indication of colloid breakthrough, but even there the retention is strong. No colloid breakthrough is observed for a 50/50 mixture when the dry density is increased to 1,800 kg/m^3.

/Wold 2003/ reports about diffusion experiments with organic colloids through MX-80 bentonite with a range of dry densities from 600 to 1,800 kg/m^3. The lignosulfonate (LS) and humic acid (HA) colloids used had an average size of 80 and < 10 nm, respectively, but the size distribution was broad. The LS and HA colloids showed diffusivities in the same range as negatively charged ions like Cl^- and I^-, which is surprising, especially for the large LS, since the mean interlayer spacing in a saturated bentonite is between ~ 5 and 10 Å. One possible explanation for lack of colloid filtration could be the presence of larger pores, the broad size distribution of the LS colloids, or transformation of the molecules during course of the experiment. The issue of organic colloid-related transport of radionuclides is one that warrents further examination.

Time perspective

The process is important for all repository timescales, but only if canisters have failed.

Natural analogues/observations in nature

No observations are available.

Handling in the safety assessment SR-Can

The concern in the safety assessment is the transport of radionuclides with colloids from a potentially failed canister, in particular fuel colloids. This transport mechanism will be neglected, provided the buffer completely envelops the canister and has a dry density of at least 1,000 kg/m^3, i.e. a saturated buffer density of at least 1,650 kg/m^3.

The effect of a loss of the colloid filtration effect will potentially be treated as a residual scenario. Transport of radionuclides in/sorbed on a colloid phase would mean that the concept of solubility limits is not valid. Radionuclide solubilties may have to be adjusted for such a scenario.

Uncertainties

Uncertainties in mechanistic understanding

As seen in the Model/Experiment section above, different types of colloids behave very differently. It is not clear why there is such a big difference between inorganic and organic colloids.

Model simplification uncertainties for the above handling in SR-Can

If the buffer density is high enough to exclude colloid transport, no model is needed in the assessment.

Input data and data uncertainties for the above handling in SR-Can

No data are used for the same reasons as are outlined above.

2.5.5 Sorption (including exchange of major ions)

Overview/general description

Radionuclides and major ions in the buffer's pore water can be bound to the surfaces of the bentonite material in several ways (see below). Together, these processes are termed sorption and are of essential importance for the function of the buffer, since they drastically affect the mobility of most radionuclides, but also of major ions that is in turn related to the evolution of the buffer. The principal mineral in bentonite is montmorillonite, which consists of octahedral alumina sheets sandwiched between tetrahedral silica sheets (2:1 clay). Such clay minerals feature two distinctly different types of surfaces, where two main types of sorption take place /e.g. Sposito 1984, Stumm and Morgan 1996/.

- The siloxane ('layer') surfaces of clay minerals are *permanent charge surfaces*. These charges can derive from isomorphous substitutions, which result in a constant negative surface charge. A macroscopically electrically neutral surface involves charge-compensating cations, and sorption takes place when compensating ions are exchanged. *Ion exchange models* have been used in soil science since the first quarter of the 20th century. Several formalisms have been developed to correct for activity changes of the exchanger as a function of the composition of the charge-compensating ions. The most common are the equivalent fraction (Gaines-Thomas, GT) and mole fraction (Vanselow) models.
- The edge surfaces of clay minerals are *variable charge surfaces*. They carry a net positive or negative surface charge depending on the species sorbed to their surfaces (potential-determining ions), often involving surface-bound OH^- groups. *Surface complexation and ligand exhange models* were established by Stumm, Schindler and co-workers in the 1970s by extending proton-binding and metal coordination chemistry in a rigorous fashion to surface chemistry. To account for the electrostatic field, the mass laws for surface equilibria often include an electrostatic correction term. The scientific basis for these corrections is derived from Electrical Double Layer (EDL) theory.

Ion exchange is the typical sorption mechanism for alkali, and alkaline-earth elements, as well as transition metals at low pH values where positive species are predominant. Surface complexation is generally the more relevant process for all reactive elements (transition metals, actinides, lanthanides, reactive anions such as carbonate). Note that both ion exchange and surface complexation take place simultaneously, but at different surfaces.

Ion exchange is an important process for the sorption of certain radionuclides (e.g. Cs, Ra, Sr) that occur in trace quantities as well as for the alteration of the total quantity of major cations. The most important factor for both processes is the cation content of the pore water, which is principally determined by the original cations in the montmorillonite's exchange positions, readily soluble minerals in the original bentonite material, and by the surrounding groundwater.

H^+ ions are bound to the edge sites of clays (as well as to ion exchange positions at very low pH), which means that pH changes can occur due to surface chemical reactions. Due to its ampholytic properties, i.e. ability to both receive and donate hydrogen ions, the montmorillonite can counteract external changes in pH /Wanner et al. 1992/.

Table 2-14 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Influence on buffer variables: Exchange reactions of major cations directly influence the surface composition of the clay minerals as well as the porewater composition. In turn, changes in the porewater chemistry may induce further changes in the bentonite composition through mineral dissolution and precipitation. The pore geometry, and thereby also the hydraulic conductivity, are not however expected to be significantly altered by ion exchange processes. This is because the volume of the buffer at reference density is so constrained that a maximum

Table 2-14. Process/variable table for the process Sorption/ion-exchane.

Variable	Does this variable influence the process?		Does the process influence this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Buffer geometry	No	(Total buffer mass considered)	No	
Pore geometry	Possibly indirectly through influence on EDL properties		Possibly indirectly, through influence on EDL properties/ swelling	
Radiation intensity	Possibly indirectly, through influence on mineral properties		No	
Temperature	Yes	Influence of temperature on sorption must be acknowledged, but effect is not clear	No	
Water content	Indirectly through porewater composition		No	
Gas content	Indirectly through porewater composition (CO2)		Possibly indirectly, through influence of Ca-exchange on carbonate equilibria	
Hydrovariables (pressure and flows)	Indirectly through porewater composition		Possibly indirectly, through porewater composition/ swelling	
Stress state	Indirectly through influence on porewater composition and EDL properties		Indirectly through influence on porewater composition and EDL properties	
Bentonite composition	Yes	Chemical data used for sorption coefficient estimates	(Surface composition)	See 2.5.6
Montmorillonite composition	Yes	Chemical data used for sorption coefficient estimates	(Surface composition)	See 2.5.6
Pore water composition	Yes	Chemical data used for sorption coefficient estimates	Yes	See 2.5.6
Structural and stray materials	Yes	Sorption on stray materials is conservatively excluded in SR-Can	Indirectly through influence on porewater composition and related mineral equilibria	

swelling of the bentonite cannot be achieved even after complete conversion to the Ca-form (or in the presence of high ion concentrations in the porewater). At saturated densities below 1,800 kg/m^3, these processes may lead to a significant reduction in the swelling pressure due to osmotic effects and a suppression of the EDL, and to an increase in the hydraulic conductivity (see Sections 2.4.1 and 2.5.8).

Influence of bentonite and porewater composition: The two most important variables with regard to radionuclide sorption and exchange of major ions are the bentonite and porewater composition. The mineralogical composition of bentonite is directly related to the amount of available sorption sites and their specific properties. The porewater composition is the result of groundwater-bentonite interaction (ion exchange, mineral equilibria) and, in turn, exerts a major influence on radionuclide sorption. Of particular importance are pH, pe, and the concentration of important ligands and competing cations.

On the other hand, K_d is clearly independent of the solid/water ratio and, therefore, of the buffer density (given that the solution composition remains constant and that the sorbing elements are not present in high enough concentrations to lead to the saturation of surface sites). Under a given set of conditions, sorption increases if the amount of bentonite (i.e. the solid/water ratio) is increased. By expressing sorption through K_d (see below), which includes the solid/water ratio, this effect is already taken into account. It appears from diffusion experiments that the apparent K_d is influenced by density, for example the K_d for caesium is halved when the density of the water-saturated system changes from 1,300 to 1,950 kg/m^3. However, this can be entirely attributed to an increase of ionic strength caused by the dissolution of impurities from an increasing mass of bentonite, and is easily reproduced by simple thermodynamic sorption models /Ochs et al. 2001/. The effect of dissolving impurities is mostly relevant in case of dilute groundwaters, less in groundwaters that are already highly mineralised.

Influence of temperature: Most experiments have been carried out at room temperature, and not enough sorption data as a function of temperature are available to clearly evaluate temperature effects. In general, a decrease of sorption with temperature would be expected, but some isolated studies /e.g. Lu et al. 2003/ indicate the opposite. Thus, an increase or decrease of the temperature is potentially of importance for sorption, but the effects within the temperature range expected in the repository are deemed to be covered with good margin by other uncertainties.

Boundary conditions

There are no particular boundary conditions to discuss for this process. The relevant boundary conditions in order to treat the process quantitatively are those of the transport processes that control the exchange of solutes between the buffer pore water and the water in its adjacent components, i.e. the boundary conditions of the processes diffusion and advection.

Model studies/experimental studies

Ion exchange as well as surface complexation are well-established processes and quantitative thermodynamic models exist for calculation of equilibrium states. The relation of these sorption processes to the different surfaces available on montmorillonite has been discussed above.

Effect of sorption on buffer properties: Conversion from sodium to calcium states by ion exchange has been modelled for deep repository conditions (taking into account all other ion exchange as well as edge site protolysis equilibria). Calculations have been carried out for expected repository conditions with respect to the content of accessory minerals (calcite, gypsum, halide) and groundwater flows /Wanner et al. 1992/. See also the processes 2.3.2 and 2.5.8.

Effect of sorption on radionuclide transport: In assessing radionuclide transport out from a repository, the sorption equilibrium is normally described as a linear relationship between the sorbed concentration and the concentration in solution, characterized by a distribution coefficient K_d, which is defined in Equation (2-25) as

$$K_d = q / C_w \qquad (2\text{-}25)$$

or in case of a batch experiment:

$$K_d = \left(\frac{C_{init} - C_{equil}}{C_{equil}} \right) \frac{v}{m} \tag{2-26}$$

where:

C_{init} is the initial aqueous concentration of a key element [mol/m^3] as measured in the reference solutions without solids

C_{equil} is the final equilibrium aqueous concentration of this element [mol/m^3]

C_w is the concentration in solution

v is the volume of the solution used for a batch experiment [m^3]

m is the mass of the solid phase used for a batch experiment [kg]

q is the sorbed concentration as mass per weight unit of solid phase

When the concentration of the species in solution is low (more specifically, at a state sufficiently far from surface site saturation), which is normally the case for radionuclides, linear approximation is justified. Note that K_d is strongly dependent on chemical conditions; and is strictly valid only for a particular set of conditions in terms of groundwater chemistry and bentonite composition. K_d can also be calculated in a straightforward fashion from the output of thermodynamic sorption models:

$$K_d\,[\mathrm{m^3/kg}] = \frac{\text{stoichiometric sum of surface species of element X [mol/kg]}}{\text{stoichiometric sum of solution species of element X [mol/m}^3\text{]}} \tag{2-27}$$

Surface complexation models with parameters from well-controlled experiments that include sufficient variations of geochemical key parameters can often be used to describe sorption's dependence on external parameters such as pH, etc, see e.g. examples in /NEA 2001/.

Time perspective

An ion exchange process in itself is fast, so the dissolution rate of other minerals and the transport rate in groundwater and bentonite pores will control the ion exchange from Na^+ to Ca^{2+}. Relevant changes in buffer properties are expected to occur on the hundred-thousand-year scale /Bruno et al. 1999/. It has to be pointed out further that modelling the conversion of Na- to Ca-bentonite by implementing ion exchange in a mixing-tank type of model, as in /Bruno et al. 1999/, is in all likelihood a pessimistic approach, in the sense that it overestimates the rate of the exchange process: To compensate the diffuse layer charge in the porespace, a certain cation concentration is required /Ochs and Talerico 2003/. While the maximum concentration of Ca is limited by the solubility of calcite or gypsum, the concentration of Na is not limited, and it can be doubted that a full conversion to the Ca-form is possible under these conditions. This is consistent with the observation that typical Ca-bentonites, such as Deponit-CaN, still contain a significant fraction of alkali elements on the exchange sites.

Sorption in the buffer is an important process for the retention of many radionuclides. The timescales that are of interest are dependent on the half-life of the individual nuclide. If the travel time through the buffer is of the same order of magnitude or longer, sorption is of great importance for the amount released. If the travel time through the buffer, including retardation from sorption, is short in comparison to half-life, the sorption process is less important.

Natural analogues/observations in nature

Many bentonite deposits contain pore water with high salinities. Investigations of effects of high salinity in natural smectites exist but have not been utilized specifically for repository-related questions. Natural analogues also offer evidence that migration of sorbing radionuclides occurred only over limited distances away from a source in clay-rich substrates /Smellie and Karlsson 1996/

Handling in the safety assessment SR-Can

Before saturation: The process is neglected.

After saturation: Ion exchange is included in the scenario specific modelling of the buffer chemical evolution for the thermal phase and the post-thermal long-term phase, see heading "Handling" for process 2.5.6.

Failed canister: Sorption is included in the modelling of radionuclide transport for the long-term phase, see heading "Handling" for process 2.6.1. Sorption is treated through element-specific K_d values derived for specific conditions (see /Ochs and Talerico 2004/ for the definition of data and associated uncertainties).

Boundary conditions: See sections referred to above.

Handling of variables influencing this process: Dependence on buffer properties as well as composition and pH of the porewater in the buffer, as resulting from bentonite-groundwater interaction, are considered in selecting sorption constants for radionuclide transport. Because of the conditional nature of sorption constants, the selected data are derived for several sets of relevant safety assessment conditions. Temperature effects are not considered explicitly, but the effects within the temperature range expected in the repository are deemed to be covered with good margin by the uncertainties associated with the selected K_d values.

Handling of variables influenced by the process: For the influence of ion exchange and surface acid-base equilibria on buffer chemical evolution, see Section 2.5.6; these processes are also taken into account in the derivation of radionuclide K_d values.

Uncertainties

Uncertainties in mechanistic understanding

Both conceptual understanding and a large quantity of measurement data exist for simplified systems. Detailed reviews of sorption processes, underlying experimental data, model results, as well as the relation to performance assessment can be found in e.g. /NEA 2001, 2005, Davis and Kent 1990/. In particular, it has been shown that thermodynamic sorption models developed for purified Na-montmorillonite can be applied to Ca-montmorillonite /Bradbury and Baeyens 1999/, and that such models give results for compacted bentonite that are compatible with diffusion data /Ochs et al. 2003/.

To date, there is no doubt that sorption processes are well understood in a quantitative way and in terms of thermodynamic description, and that this understanding can be used to make educated predictions of K_d values to be used in safety assessment calculations. However, there is a clear lack of data for understanding and predicting the influence of some important variables (such as dissolved carbonate concentration or competition by major cations) on radionuclide sorption, and this has to be taken into account in evaluating uncertainties of K_d values /Ochs and Talerico 2004/. In case of some radionuclides, the underlying thermodynamic database is insufficient to quantitatively evaluate their behaviour for different conditions.

Model simplification uncertainties for the above handling in SR-Can

As pointed out above, the K_d concept for radionuclide transport modelling is basically justified under conditions far from surface saturation, which can be expected in the case of diffusion-limited radionuclide migration in a bentonite buffer. At the same time, it is clear that K_d is a highly conditional parameter in terms of chemical conditions (pH, ionic strength, etc) and has to be derived for each set of conditions. This was done in case of the data selection for SR-Can using a semi-quantitative, traceable procedure to transfer K_d data from experimental to safety assessment-specific conditions /Ochs and Talerico 2004/. For several elements, it was possible to use state of the art thermodynamic sorption models to derive K_d values for the specified conditions. The model-derived data were in all cases within the uncertainty range of the values that had been derived using the semi-quantitative conversion procedure. This strongly suggests that for the specified conditions, use of a sorption model and direct use of recommended K_d values would lead to consistent results (i.e. use of K_d would not introduce additional uncertainties, as long as the conditions remain constant). To avoid potential problems related to the direct use of K_d in cases where conditions may vary to some degree (or to avoid re-derivation for each condition), thermodynamic sorption models could be directly coupled with transport codes (see Section 2.5.3). Again, for many radionuclides not enough systematic sorption data for the relevant conditions are available to date to develop or sufficiently constrain thermodynamic models.

As long as the bentonite buffer can be expected to represent a homogeneous geochemical compartment, no spatial variability needs to be taken into account.

Input data and data uncertainties for the above handling in SR-Can

Input data to SR-Can are K_d values to be directly used in consequence calculations. K_d values for radionuclides valid for MX-80 under various conditions, as well as the associated uncertainties are given in /Ochs and Talerico 2004/, from which data for consequence calculations are chosen in the SR-Can data report.

No sorption data are available for Deponit-CaN. However, based on the relatively similar composition of MX-80 and Deponit-CaN, it can be assumed that radionuclide sorption will be similar under reference conditions (see /Ochs and Talerico 2004/): Based on the CEC of Deponit-CaN (70 meq/100 g) and MX-80 (75 meq/100 g), sorption can be expected to be only negligibly smaller in case of Deponit-CaN. Calculations of the porewater composition in Deponit-CaN with the model of /Wanner et al. 1992, Wieland et al. 1994/ indicate that porewater pH in Deponit-CaN at a dry density of 1,590 kg/m^3 may be slightly lower (7.11 instead of 7.37 as in case of MX-80). Similarly, concentrations of major ligands (carbonate, sulphate) differ by less than a factor of 3 between the porewater compositions calculated for the two bentonites. All of these variations fall well within the respective parameter ranges that had been considered in the selection of input data /Ochs and Talerico 2004/ to take into account uncertainties in the composition of the contacting groundwater. Moreover, it is shown in /Ochs and Talerico 2004/ that the conversion of MX-80 from the Na- to the Ca-form would decrease K_d of Cs (which sorbs only via ion exchange and is therefore sensitive to the composition of exchangeable ions) by less than a factor of two. Based on all of the above evidence, uncertainties in K_d values due to a variation in bentonite composition can be expected to fall within the ranges already indicated in the data report.

2.5.6 Alterations of impurities

Overview/general description

The buffer material consists not only of montmorillonite, but also other accessory minerals as well as impurities. In the repository environment, these can be dissolved and sometimes reprecipitated depending on the prevailing conditions.

Precipitation of carbonates and sulphates in the areas nearest to the canisters may lead to the formation of a porous contact zone between the buffer and the canister surface and an increase in the strength of the buffer. When the thermal period is over and temperature gradients no longer exist to any substantial extent in the buffer, it is likely that the previously precipitated solids will be redissolved to some degree and then diffuse in ionic form out through the buffer. Precipitation of silica may reduce the swelling potential, as well as decrease the bentonite porosity.

The composition of MX-80 and Deponit CA-N can be found in Table 1-2.

The carbonate and pyrite contents are of decisive importance for pH, Eh and alkalinity in the near field. Bentonite also contains small quantities of gypsum ($CaSO_4{\cdot}2H_2O$), which may be of importance in an early phase during the high temperature transient.

Evaporation of incoming groundwater during the saturation phase in the warmer parts may lead to different concentration of dissolved elements at different positions in the buffer.

The accessory minerals in bentonite are either stable or metastable in the environment where they were originally mined. In the repository, however, they will be exposed to a fluid that differs in some respects from that on the original site, in terms of both composition and temperature. Most accessory minerals in the bentonite are nevertheless stable in the granitic groundwaters prevailing in the Fenoscandian shield. There are, however, some dissolution-precipitation processes that are important:

Calcite dissolution: Calcite is stable in groundwater. In the bentonite, however, the ion exchange process will compete for the free calcium ions. The reaction

$2XNa + Ca^{2+} \leftrightarrow X_2Ca + 2Na^+$

competes with

$Ca^{2+} + HCO_3^- \leftrightarrow CaCO_3(s) + H^+$

The carbonate contents of the groundwaters that may be encountered are sufficiently low for the ion exchange process to dominate and calcite will be dissolved. This will entail a net proton consumption, i.e. an increase in pH. The water flux in the buffer is very low, and the reactions are close to equilibrium.

Siderite dissolution and iron hydroxide precipitation: The presence of pure siderite or ankerite, a mixed calcium-iron carbonate is of paramount importance for the redox control of the system through the following reaction

$FeCO_3(s) + \frac{1}{4}O_2(aq) + 2\frac{1}{2}H_2O \leftrightarrow Fe(OH)_3(s) + HCO_3^- + H^+$

Siderite oxidation leads to an increase of iron in solution allowing the precipitation of iron (III) hydroxides and thus controlling the redox of the system. However, during the early stage, when high temperatures are expected in the buffer, hematite would be the stable iron (III) phase instead of iron (III) hydroxide, leading to the precipitation of hematite close to the canister and increasing the strength of the buffer.

Pyrite oxidation/dissolution: Pyrite is also stable in groundwater. However, penetrating oxygenated water can oxidise pyrite in accordance with

$2\ FeS_2(s) + 7\frac{1}{2}O_2(aq) + 7H_2O \leftrightarrow 2Fe(OH)_3(s) + 4SO_4^{2-} + 8H^+$

Pyrite oxidation releases protons and can thereby lower the pH, but this is buffered by the dissolution of calcite previously discussed. There is enough pyrite in the buffer to consume all initial oxygen left after closure of the repository. The air content in bentonite buffer is 12% by volume /SKB 2004c/, corresponding to 1.9 moles of oxygen gas per cubic meter of bentonite, thus 0.51 moles of pyrite in 1 m^3 of bentonite are needed to consume all this oxygen, which is equivalent to a pyrite content of 0.004% by weight, which is 20 times lower than the pyrite content of MX-80 bentonite or 125 times lower than the pyrite content of Deponit-CaN bentonite. The quantity is also sufficient to prevent any penetrating oxygenated water from coming into contact with the canister for hundreds of thousands of years. However, as this process is kinetically driven, it is likely that pyrite oxidation exerts a minor effect on the redox of the system, which will be controlled by the iron carbonate dissolution process.

Pyrite is a source of a sulphides that could act as a corrodant on the copper canister. Under reducing conditions pyrite dissolves as:

$FeS_2(s)+H^+ \leftrightarrow Fe^{2+} + HS^- + S^0$

The concentration of HS^- is an important parameter for the canister corrosion.

Dissolution of calcium sulphates: Calcium sulphates (gypsum and anhydrite) and calcite have lower solubility at high temperatures. At an early stage, when the canister temperature is high, it is possible that they will be dissolved in the colder portion of the buffer and precipitate on the canister surface.

Precipitation/dissolution of silica: The largest portion of the impurities in the bentonite consists of quartz and feldspars. Feldspars are not stable in the repository environment, although the kinetically driven dissolution is a relatively slow process that is accompanied by the precipitation (or replacement) of clay minerals, i.e. kaolinite. The low water flux in the buffer is likely to minimise the kinetic dissolution of feldspars. Quartz is normally stable in the natural repository environment, but its solubility increases with increasing temperature. Silica will dissolve due to high temperature close the canister and will be transported by diffussion outwards into the colder parts where precipitation may take place. In the Buffer Mass Test in Stripa, the buffer was analyzed with respect to the distribution of silicon, but no definite conclusion could be drawn regarding possible enrichment in the coldest part /Pusch 1985b/.

Most of the conceivable processes are in themselves well known and can be modelled for less complex systems. However, conditions in the buffer, as far as transport and reaction kinetics are concerned, are not fully understood for all processes. Transport of solutes can take place in different forms and cannot be fully described at present. In particular, modelling problems remain during the water saturation phase, when water is transported both in vapour and liquid form. Modelling of the system must therefore be coupled to the THM processes that proceed in parallel with transport and reaction kinetics.

Silicon is the most common element in the buffer and occurs in a number of different minerals and phases. The following processes are not fully understood:

- release of silica by dissolution from different minerals,
- transport of dissolved silica driven by the prevailing temperature gradient,
- precipitation of silicon minerals.

Precipitation of silica is particularly complex, since it is dependent on several interacting factors and since several conceivable forms occur, both crystalline and amorphous.

The greatest uncertainty concerns the scope of cementation processes as a consequence of dissolution, transport and precipitation of silicon or aluminosilicate minerals. The scope and consequences of cementation cannot be predicted with reasonable certainty today.

Table 2-15 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Boundary conditions

There are no particular boundary conditions to discuss for these processes. The relevant boundary conditions in order to treat the process quantitatively are those of the transport processes that control the exchange of solutes between the buffer pore water and the water in its adjacent components, i.e. the boundary conditions of the processes diffusion and advection.

For alterations of impurities, the exchange of a number of solutes like sodium and calcium ions, carbonate and oxygen is relevant.

Table 2-15. Process/variable table for the process Alteration of impurities.

Variable	Does this variable influence the process?		Does the process influence this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Buffer geometry	Yes	(Total buffer mass considered)	No	
Pore geometry	Yes	Determines the diffusivity, see 2.5.3	Precipitation-dissolution of minerals	The effect of “cementation” is discussed
Radiation intensity	Only very high radiation fields could influence the processes.		No	
Temperature	Temperature highly influences the extent of precipitation/dissolution of secondary minerals.	Temperature and temperature gradient in included in the chemical model	No	
Water content	Yes, could affect concentrations	However, the chemical model assumes saturated conditions	Precipitation-dissolution of accessory minerals modifies the porosity.	The effect on the overall porosity is small and not accounted for
Gas content	A secondary effect from water content variations.		Yes	Dissolved gases are included in the model
Hydrovariables (pressure and flows)	Yes	Darcy flow is included in the model	No	
Stress state	Yes	Partial pressures are included in model	Yes	The results from the model is evaluated to consider effects on swelling pressure
Bentonite composition	Yes	Composition data is considered in model	Yes	The evolution of the composition is calculated with the model
Montmorillonite composition	Yes	Composition data is considered in model	Yes	The evolution of the composition is calculated with the model
Pore water composition	Yes	Composition data is considered in model	Yes	The evolution of the composition is calculated with the model
Structural and stray materials	Yes	See 2.5.9	Secondary mineral formation/dissolution may influence the alteration of structural components. This is particularly true for sulphates.	The fate of structural material is not evaluated in SR-Can

Model studies/experimental studies

Hydrothermal tests with purified standard bentonite (SWY-1) heated to 150–200°C have shown that cooling leads to precipitation of silicon compounds in various forms. The precipitation is assumed to cause cementation effects, including a strength increase, which has been demonstrated in several laboratory investigations /Pusch and Karnland 1988, Pusch et al. 1991/.

According to these investigations, the extent of the precipitations is dependent on the temperature. At the highest temperature in the buffer (90°C), the cementation was not of such a great extent that it could be regarded as problematic. The tests were carried out without a temperature gradient, which cannot be regarded as pessimistic conditions.

Precipitation of sulphate and carbonate could be observed in one-year experiments with hydrothermal treatment of MX-80. XRD analyses indicated that sulphates and calcite had gone into solution and been transported to the hot iron surface, where they had been precipitated. Based on a geochemical model /Pusch et al. 1993/, it is also probable that feldspars dissolved and that quartz was enriched at the colder boundary. In the Buffer Mass Test in Stripa (max 90°C), the buffer was analyzed with respect to the distribution of silica, but no definite conclusion could be drawn regarding possible enrichment in the coldest part /Pusch 1985b/. However, the study of cooling-related precipitation of silica predicted by the Grindrod/Takase/Pusch model was confirmed by the Kinnekulle case /Pusch et al. 1998/.

In the LOT tests at Äspö HRL, buffer material is exposed to high temperature gradients (maximum 130 to 80°C over a 10 cm distance). Material from the one year tests was analysed at 25 positions with respect to element distribution and rheological properties. No significant gradients were found for silica content. The tensile strength was slightly reduced and the tensile strain was slightly increased, which shows that no cementation had taken place in the major part of the buffer material. However, precipitation of mainly gypsum was found in a 1–2 mm thick rim around the copper tube. The ongoing five-years tests are expected to give information on whether the precipitation is an effect of evaporation of the inflowing water as a part of the saturation process, or if the process continues also after full water saturation.

Several laboratory investigations have been carried out for the purpose of studying the distribution of readily soluble ions in the buffer's pore space after water uptake against a temperature gradient. Effects of the clay's density, degree of saturation, testing time, open or closed conditions, and ion content and pressure in the ambient water solution have been investigated. The experimental results show that the enrichment of solutes is insignificant in specimens with high clay density, and that a high original water content and high ambient water pressure reduce the enrichment in specimens with lower density /Karnland 1995/. Similar studies are currently being conducted in field tests in Äspö (the LOT project) /Karnland et al. 2000/, and in laboratory experiments under the auspices of ENRESA.

Several geochemical models have been developed in order to predict the long-term behaviour of the buffer under repository conditions. Some of the models are based on a mixing tank concept /Wanner et al. 1992, Bruno et al. 1999/ where the thermal stage has not been considered. Other models are reactive transport based models where the thermal stage is considered /Arcos et al. 2000/. All these models suggest that cation exchange is the dominant process in the buffer resulting in a direct control on the calcite precipitation-dissolution, thus buffering the pH of the system. Also the effect protonation-deprotonation of montmorillonite edge sites can play a role on the pH buffering. However, earlier models /Bruno et al. 1999, Arcos et al. 2000/ indicate that calcite equilibrium is the main process buffering pH, and only if calcite is exhausted edge sites will be able to buffer pH in the system. The redox buffering capacity of the bentonite is somewhat controversial according to these models. Some of the models predict the redox buffering is due to pyrite oxidation and iron (III) hydroxide precipitation; whereas other models pointed to the iron carbonate (siderite) dissolution and iron (III) oxy-hydroxides as the redox buffering capacity of the system.

An additional geochemical model for use with the LOT experiment at Äspö /Arcos et al. 2003/ has been developed and has generated results similar to those obtained in previous models. Unfortunately there are still no experimental data to compare with. It should also be noted that when comparing the new modelling results with experimental data /Domènech et al. 2004/ some disagreements have been observed. It is likely that these differences are due to the uncertainty associated to the initial conditions selected for the model. The initial conditions for the model are being revised in the framework of the LOT project.

Natural analogues/observations in nature

Development of salt crusts in arid regions resembles in principle certain conditions during the water saturation phase. Direct SKB-related studies have not been conducted, but a large body of literature exists on the subject.

Silica precipitation occurs at a large number of places where hydrothermal transformation of bentonite has taken place. Numerous scientific articles have been published, some directly linked to repository questions, see for example /Pusch et al. 1998/.

At present, SKB is involved in the study of a bentonite natural analogue in Spain, the BARRA project, under the coordination of ENRESA. Two processes are being studied in this natural system: 1) the changes in the bentonite induced by long time exposition to very high salinity environment, and 2) the thermal effect induced by a sub-volcanic intrusion on the bentonite properties The initial results from this study indicate that exposure to very high salinities does not alter the properties of the bentonite.

Time perspective

The chemical precipitation/dissolution processes are most important at an early stage when temperature and temperature gradients are high and oxygen remains in the repository tunnels. At later stages, most of the processes go towards equilibrium. The accessory minerals in the bentonite are, however, important also over timescales of hundreds of thousands of years if the chemistry in the repository should be disturbed for some reason; both pH and Eh are buffered effectively by the accessory minerals that are common in different bentonite materials.

Handling in the safety assessment SR-Can

Model: Before saturation: Geochemical processes will be the same both before and after saturation phases. This is just a matter of water flow and solutes transport, although the extent of the reactions (dissolution/precipitation) will be different.

After saturation: The process is included in the scenario specific modelling of the buffer chemical evolution for the thermal phase and the post-thermal long-term phase. This modelling includes, in addition to alterations of impurities, also the processes diffusion (Section 2.5.3), ion exchange (Section 2.5.5) and aqueous speciation and reactions (Section 2.5.7). In formulating initial conditions, the initial intrusion of groundwater during buffer saturation should be considered if that has a relevant influence on the initial conditions. The main model will be a 2D reactive transport model based on the geochemical models of the LOT experiment /Arcos et al. 2003, Domènech et al. 2004/. The model handles advective flow in a fracture in granite intersecting the deposition hole, diffusive transport in the bentonite, dissolution-precipitation of main bentonite accessory minerals, cation exchange in the bentonite, protonation-deprotonation reactions in the smectite fraction and precipitation of favoured secondary phases in both bentonite and granitic fracture. Prior to application in SR-Can, the reactive transport model will be validated by comparing its results with experimental data from the LOT test.

In addition, a simplified mixed tank model embedded in the near-field evolution model /Hedin 2004/ will be used for preliminary calculations and to study sensitivities to input data.

Failed canister: In the case of a failed canister, vast amounts of metallic iron, originating from the corroding cast iron canister insert, will be added to the geochemical system. This will be included in the model mentioned above, in a dedicated calculation case.

Boundary conditions: Main model: The diffusive transfer of species between the flowing water and the bentonite is explicitly modelled. The near-field evolution model uses the Qeq concept to handle the boundary conditions. This is sufficient to estimate a general timescale on which the evolution occurs.

Handling of variables influencing this process: The modelling is in itself a coupling of the four (groups of) processes mentioned above and is thus a coupled modelling of most of the significant long-term chemical processes. A large number of the variable influences related to the chemical conditions (pore water composition, montmorillonite composition, bentonite composition) are also included.

Handling of variables influenced by the process: The geochemical conditions in the near-field as a function of time and space will be calculated.

The changes in the buffer accessory mineral content as a consequence of the thermal stage has been modelled, but not validated through a comparison with experimental and/or natural analogue data. This makes it difficult to ensure that changes due to the thermal stage are minor or that these results should be assumed to be the initial conditions for the low temperature stage.

In addition to the processes discussed above, the behaviour of silica and clay minerals and their effect on cementation will be addressed by performing some scoping calculations considering the present knowledge on kinetic dissolution-precipitation of smectite, silica-phases and the precipitation of alternative clay minerals (kaolinite and/or illite). These scoping calculations would give some qualitative information on the relative importance of these processes and the effect on bentonite properties, i.e. porosity changes. See also Section 2.5.9.

Uncertainties

Uncertainties in mechanistic understanding

Some critical uncertainties remain concerning the mechanistic understanding of the processes that control the redox state of the bentonite system. It is not clear yet to what extent pyrite and/or siderite are the main redox controlling phases, although either process, or their combination, will scavenge the remaining oxygen in the near field. This should be discerned by comparative modelling of pyrite and siderite kinetic availability.

In addition, most of the secondary precipitation/dissolution processes that are temperature driven are thermodynamically controlled. Hence, there is no need for a detailed mechanistic understanding. However, some of the silicate transformations are kinetically controlled and their mechanistic understanding in compacted bentonite conditions is poor. This is mainly related to clay mineral transformations (dissolution of smectite and precipitation of illite and/or kaolinite). Although these reactions occur at a very slow rate, their effect on the overall geochemical evolution is not yet clear.

Model simplification uncertainties for the above handling in SR-Can

Secondary dissolution and precipitation processes have not been fully implemented in a coupled model of buffer evolution. The processes are only considered when required for the definition of critical master variables in the system (pH and pe). A possibility could be to couple the THM processes occurring with the key chemical processes that will control the geochemical evolution of the buffer system.

There are a number of accessory minerals, such as silicates other than silica, which are not included in the models, as most of them tend to dissolve at a very slow kinetic rate. Other silicates (usually clay minerals) precipitate at similarly slow rates. However, the dissolution-precipitation processes involving these two groups of minerals could affect the stability of montmorillonite as well as the chemical composition of the buffer pore water, thus affecting the chemical long-term evolution of the buffer. See also Section 2.5.9.

There is no model accounting for the dissolution/precipitation of accessory minerals during the water saturation stage of the buffer. As water flux will be faster than when the buffer is water saturated and the buffer composition will be far from equilibrium with incoming water, some changes will occur faster. These changes will account for step compositional gradients in the buffer and changes in porosity as accessory minerals dissolve and/or precipitate, leading to changes in hydraulic properties of the buffer. Thus, modelling of the system must therefore be coupled to the THM processes that proceed in parallel with transport and chemical reactions. A submodel dealing with the saturation stage of the bentonite will, at least, give an idea on the magnitude of theses changes.

Input data and data uncertainties for the above handling in SR-Can

Key thermodynamic data are well established and therefore reliable. The main uncertainties remain in the definition of the kinetically controlled processes. These are linked to the mechanistic uncertainties previously mentioned.

Proper data for surface reactions (i.e. cation exchange and edge site reactions) is of paramount importance for the correct assessment of the bentonite behaviour. Two types of information are needed for geochemical modelling: i) Cation occupancy of the CEC and protonation state of the smectite surface, and ii) Exchange and protonation-deprotonation constants. The main uncertainty associated with these data is related to the experimental conditions used for their determination (i.e. low bentonite density and high solid/liquid ratios). Recent experiments have addressed this problem, however there is still a large uncertainty related to the determination of cation exchange constants and their variation as a function of bentonite density. These data and the associated uncertainties will tentatively be handled in the SR-Can data report.

2.5.7 Aqueous speciation and reactions

When the buffer is saturated, the water content is about 40 vol%. The composition of this water will be determined by the composition of the pore water present at deposition, of the composition of groundwater on the site, reactions with the buffer and canister material and the impurities in the bentonite. Within the aqueous phase chemical reactions will take place and the final composition of the water can be determined with thermodynamics and kinetics. Usually aqueous speciation reactions are fast, i.e. controlled by thermodynamics. Examples of this are reactions like:

$HCO_3^- \leftrightarrow CO_3^{2-} + H^+$ and $HS^- + H^+ \leftrightarrow H_2S(aq)$

Overview/general description

Table 2-16 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Boundary conditions

By definition, this process takes place in the pore water. The boundary conditions will be the canister, the groundwater, the bentonite and the impurities.

Model studies/experimental studies

Direct measurements of the porewater composition in compacted bentonite are virtually impossible. Limited amounts of water can be squeezed out under high pressure, but the composition of that water may not be representative of the porewater. The amount of non-sorbing elements with high solubility can be measured by total dispersion of the bentonite sample in water, still this only gives the total amount and reveals nothing about the speciation in the bentonite.

Modelling of the chemical composition/speciation of the porewater is done with an integrated model for the chemical evolution in the near field. This is described in 2.5.6. Speciation of radionuclides is discussed in upcoming process report for the Fuel, See also the process report for SR 97 /SKB 1999/.

Table 2-16. Process/variable table for the process Aqueous speciation and reactions.

Variable	Does this variable influence the process?		Does the process influence this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Buffer geometry	No		No	
Pore geometry	No		No	
Radiation intensity	(Yes)	See 2.5.12	No	
Temperature	Yes	Included in model see 2.5.6	No	
Water content	No		No	
Gas content	No		No	
Hydrovariables (pressure and flows)	Yes	See 2.5.6	No	
Stress state	Yes	See 2.5.8	Yes	See 2.5.8
Bentonite composition	No		No	
Montmorillonite composition	Yes	See 2.5.9	Yes	See 2.5.9
Pore water composition	Yes	See 2.5.6	Yes	See 2.5.6
Structural and stray materials	No		No	

Natural analogues/observations in nature

Not applicable.

Time perspective

The process is important for all repository timescales.

Handling in the safety assessment SR-Can

Before saturation: Geochemical processes will be the same before and after saturation. This is just a matter of water flow and solutes transport, something to be considered in other sections.

After saturation: The process is included in the scenario specific modelling of the buffer chemical evolution for the thermal phase and the post-thermal long-term phase. This is described in Section 2.5.6.

Failed canister: In the case of a failed canister, vast amounts of metallic iron, originating from the cast iron canister insert, will be added to the geochemical system. This will be included in the model mentioned above, as a dedicated calculation case.

Boundary conditions: See Section 2.5.6.

Handling of variables influencing this process: The modelling is in itself a coupling of the four (groups of) processes mentioned above and are thus a coupled modelling of most of the significant long-term chemical processes. A large number of the variable influences related to the chemical conditions (pore water composition, montmorillonite composition, and bentonite composition) are also included.

Handling of variables influenced by the process: The chemical composition of the pore water is calculated. The result may have influence on process 2.5.8 and 2.5.9.

Uncertainties

Uncertainties in mechanistic understanding

The model assumes that the chemistry in porewater is identical to the chemistry in liquid water. The effect of the bentonite surface and structure is not included (except the ion-exchange). It is not clear if or how this will affect the chemistry. See also Section 2.5.8.

Model simplification uncertainties for the above handling in SR-Can

See Section 2.5.6

Input data and data uncertainties for the above handling in SR-Can

See Section 2.5.6

2.5.8 Osmosis

Overview/general description

A classical view of osmosis, as shown in Figure 2-17 may be used in order to illustrate the conditions in a bentonite buffer. The two sides of the water system are divided by a semi-permeable membrane only permeable to water molecules. If salt is added to the left side, the water activity is reduced and a transport of water from right to left will take place. The left water table will thereby rise and a hydrostatic pressure develops (a). If salt is now added to the right side, there will be a leveling of the water tables on both sides (b). If the volume change, in the first place, is instead prohibited by force, a pressure will rise in the salt solution (c), corresponding to the previous hydrostatic pressure. Introduction of salt into the right hand side of the membrane will lead to a drop in pressure. A complete drop of pressure will evidently take place when the two concentrations are equaled (d).

The analog to bentonite buffer is that the left side of the system represents the bentonite and the right side an external groundwater solution (Figure 2-18). An external solution would reduce the pressure produced by the clay, to an extent equal to the osmotic pressure of the solution, if no ions could pass into the clay. A sodium chloride concentration of around 1.7 M (10% by weight) would then result in a complete loss of swelling pressure in a KBS-3 buffer. On the other hand, if ions could pass freely into the clay, then the final conditions would be equal concentrations on both sides and no effect on swelling pressure would be found, neither of which is in agreement with experimental results. Laboratory experiments show that ions from the external solution do pass into the clay to a certain extent, and the difference in concentration between external and introduced ions leads to a drop in the swelling pressure /Karnland 1997/.

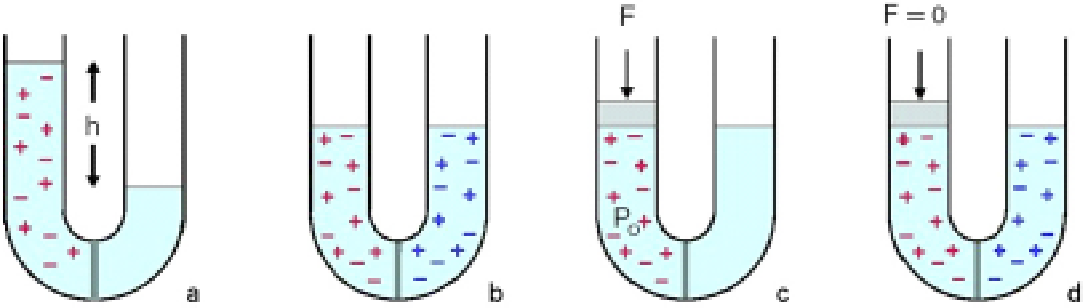

Figure 2-17. The basic principles of osmosis as an analogue to bentonite swelling pressure.

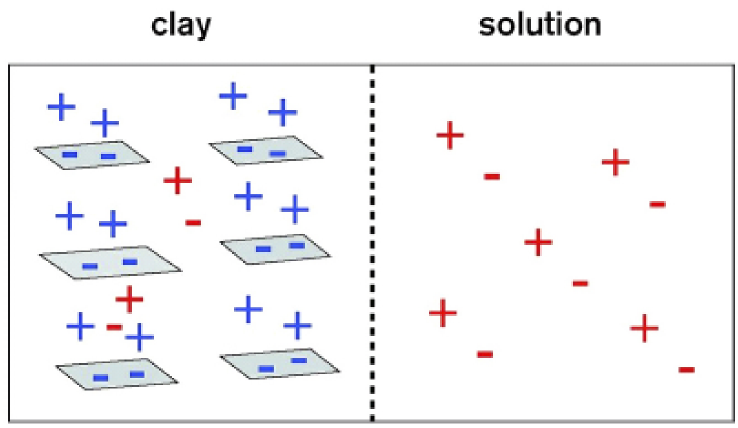

Figure 2-18. *Principle drawing of the clay-water-ion system. Clay mineral flakes and charge compensating cations on the left side, and sodium and chloride ions on both sides of a semi-permeable membrane (buffer-rock interface), which is permeable to dissolved ions and water, but not to the individual montmorillonite layers.*

The conditions in the bentonite/groundwater system are typical for what is often referred to as a Donnan equilibrium system /Donnan 1911/. The equilibrium is characterized by one ion that cannot freely diffuse in the system, usually because of its large size. The conditions lead to an unequal distribution of ions that are diffusible across a membrane separating the two volumes. In a repository, the non diffusible ions correspond to the individual montmorillonite mineral layers, which are electrically charged and have a restricted mobility because of their relatively large size compared to the induced mean pore-size, see Section 2.5.3, and the membrane corresponds to the rock interface where dissolved electrolyte ions may pass but not the montmorillonite layers (Figure 2-18).

The condition for equilibrium is that the chemical potentials are equal on both sides of the membrane for all components that can permeate. Since the macro-sized mineral layers cannot pass the membrane, an equilibrium will be established only for ions in the saturating solution and the montmorillonite charge compensating cations. Ideally, for sodium montmorillonite and a sodium chloride solution this will only be Na^+ and Cl^-. The conditions of electrical neutrality in the entire system are:

$$0 = z \cdot C_m + C_{Cl-} - C_{Na+} \qquad (2\text{-}28)$$

where z is the valence of the macromolecule, C_m, C_{Na+} and C_{Cl-} is the concentration of the macromolecules, sodium ions and chloride ions, respectively. In terms of ion activity the equilibrium condition for the diffusible ions will be:

$$\{Na^+_c\}\{Cl^-_c\} = \{Na^+_e\}\{Cl^-_e\} \qquad (2\text{-}29)$$

where the indices c and e refer to the clay-water system and to the surrounding electrolyte, respectively. The $\{Na^+_c\}$ factor is the sum of the concentration of original charge compensating ions $\{Na^+_{cc}\}$ and introduced electrolyte ions $\{Na^+_{ie}\}$. Local electrical neutrality has to be established thus $\{Na^+_e\} = \{Cl^-_e\}$ and $\{Na^+_{ie}\} = \{Cl^-_{ie}\}$ which give:

$$(\{Na^+_{cc}\}+\{Na^+_{ie}\})\ \{Na^+_{ie}\} = \{Na^+_e\}\ \{Na^+_e\}) \qquad (2\text{-}30)$$

Rearranging gives the introduced sodium ions:

$$\{Na^+_{ie}\} = \frac{-\left[\{Na^+_{cc}\} \pm \sqrt{\{Na^+_{cc}\}^2 + 4 \cdot \{Na^+_e\}^2}\right]}{2} \qquad (2\text{-}31)$$

Consequently, it is possible to calculate the activity of sodium ions introduced into the clay-water system if the activity of the original cations {Na^+_{cc}} in the clay and the activity of the ions in the external solution {Na^+_e} are known. The resulting drop in swelling pressure can be approximately calculated since the activity of both the groundwater and the interlayer cations can be determined /Karnland et al. 2002/. Figure 2-19 shows measured and calculated results for the above conditions. The same principle may be applied to divalent ions, which leads to a more complicated expression, but both measured and calculated values for calcium show similar osmotic effects as for sodium.

Table 2-16 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Boundary conditions

The process occurs at the interface between the bentonite and the outer solution. Generally, this is the rock/bentonite interface, but could also occur at the bentonite/canister interface in the case of a defected canister.

Model studies/experimental studies

The first preliminary study has been reported in SKB TR 97-31. A comprehensive model and experimental study of MX-80 bentonite converted to a pure sodium state has been made by SKB and is reported /Karnland et al. 2002/. An experimental study of the two reference bentonites MX-80 and Deponite-CAN is ongoing. Results for natural material, after conversion to pure sodium conditions, and after conversion to pure calcium conditions are presently available /Karnland et al. 2006/.

Time perspective

The process is relevant for all timescales in the lifetime of the repository. The effect of a change in groundwater salinity is expected to result in an almost instantaneous response in swelling pressure.

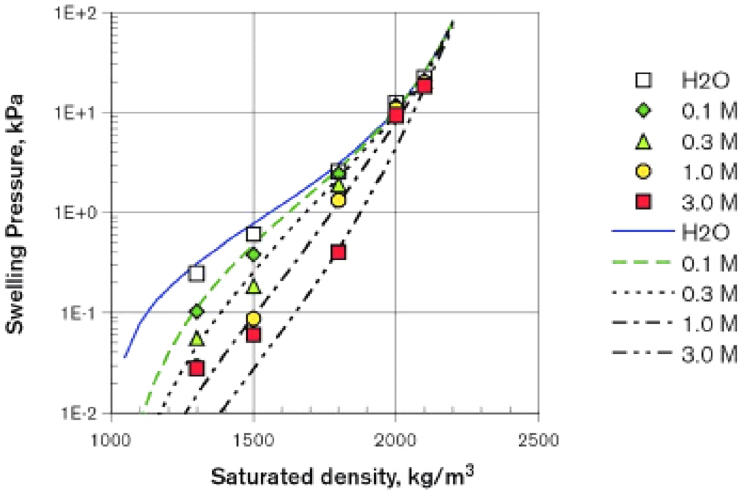

Figure 2-19. *Measured (squares) and calculated (lines) swelling pressure versus clay density for different concentrations in an NaCl solution in equilibrium with the Na-montmorillonite. Legends show external solution concentration in mole/L.*

Table 2-16. Process/variable table for the process Osmosis.

Variable	Does this variable influence the process?		Does the process influence this variable?	
	Influence present?	**Handling of influence?**	**Influence present?**	**Handling of influence?**
Buffer geometry	No		Indirect through stress state	
Pore geometry	Indirect through stress state		Indirect through stress state	
Radiation intensity	No		No	
Temperature	Yes	Data is lacking on the temperature effect on this process. The effect is expected to be of limited concern	No	
Water content	Yes	See 2.3.1	Indirect through stress state	
Gas content	No		No	
Hydrovariables (pressure and flows)	Determines availability of water	Only water chemistry is evaluated (conservatively)	Affects hydraulic conductivity	The effect of salinity is evaluated
Stress state	The initial swelling pressure determines the effect of the process	The effect of salinity is evaluated	Yes	The effect of salinity is evaluated
Bentonite composition	No		No	
Montmorillonite composition	The initial composition determines the effect of the process	The effect of salinity is evaluated	No	
Pore water composition	Yes	The effect of salinity is evaluated	(Yes) to a small extent	Only effects on the buffer itself are considered
Structural and stray materials	No		No	

Natural analogues/observations in nature

Osmotic effects related to clay are discussed in several articles, but they are only peripherally relevant for repository conditions. Osmotic fluid pressure effects are recently discussed in /Neuzil 2000/.

Handling in the safety assessment SR-Can

The osmotic swelling pressure effects are handled either by direct application of empirical data for relevant, scenario-specific conditions or by using the near-field evolution model, in e.g. calculations of buffer displacement as a result of swelling in saline groundwaters.

Model: The relationship presented above will be used to estimate swelling pressure and hydraulic conductivity for the buffer.

Boundary conditions: The important boundary condition for this process is the composition of the groundwater.

Handling of variables influencing this process: The montmorillonite composition and the groundwater/porewater composition are directly included in the model.

Handling of variables influenced by the process: The buffer swelling pressure and hydraulic conductivity will be calculated.

Uncertainties

Uncertainties in mechanistic understanding

The process is based on well-established theories and generally well understood. How they can be applied to buffer conditions is however not clear in detail and quantification is not precise. The main remaining issue is the actual pore geometry, which is not determined in detail. At buffer conditions this may be relevant at very high groundwater concentrations. For low clay densities, this issue is relevant for all groundwater concentrations.

Model simplification uncertainties for the above handling in SR-Can

The ion equilibrium model for predicting swelling pressure is based on the assumption that the system is relatively homogenous with respect to pore geometry. This assumption is supported by calculations of swelling pressure in electrolyte free montmorillonite by use of the Poisson-Boltzmann equation. If this assumption is not correct then the swelling pressure may decrease due to homogenization of the pore geometry with time.

Data uncertainties for the above handling in SR-Can

The input data to the model is the activity of ions in the groundwater, and the activity of the interlayer cations in montmorillonite. The model is relatively insensitive to the difference in activity and concentration for groundwater, and standard methods may be used for calculating this activity. The activity of the interlayer cations is not possible to determine by standard methods (Debey-Hückel, Davis, Pitzer etc). Uncertainties therefore still remain as to how this activity should be treated in a conservative way. A very conservative possibility is to use the same activity constants for interlayer ions as for the groundwater conditions. This will however not be applicable to the tunnel backfill material.

2.5.9 Montmorillonite transformation

Overview/general description

The advantageous physical properties of the buffer, e.g. swelling pressure and low hydraulic conductivity, are determined by the interaction between water and the montmorillonite mineral in the bentonite, see Sections 2.4.1 and 2.5.1. Other minerals with the same principal structure but different layer charge occur in nature, Figure 2-20. If the layer charge is near zero (pyrophyllite), there is virtually no interaction with water, which results in radically different properties than for montmorillonite. Minerals with higher layer charge and thereby more balancing cations may lead to greater interaction with water. However, the cations can be bound to the mineral surfaces if the layer charge is sufficiently high, and the interaction with water again ceases. The critical layer charge for cation fixation is dependent on the properties of the charge compensating cations. Layer charges above 1.2 unit charges per $O_{20}(OH)_4$, and potassium as counter-ion may result in no water interaction and fixation of the basal distance to around 1 nm. The end minerals, in which there is virtually no interaction with water, has 2 unit charges per $O_{20}(OH)_4$ for the potassium and sodium minerals (micas), and 4 units for calcium minerals (brittle micas).

Transformation from montmorillonite to illite is well documented in several different geological formations, and has been reproduced under laboratory conditions. However, illite mineralogy is not well defined, and may be seen as a transition material from montmorillonite to mica minerals. All intermediate stages from swelling to non-swelling material may be found (mixed

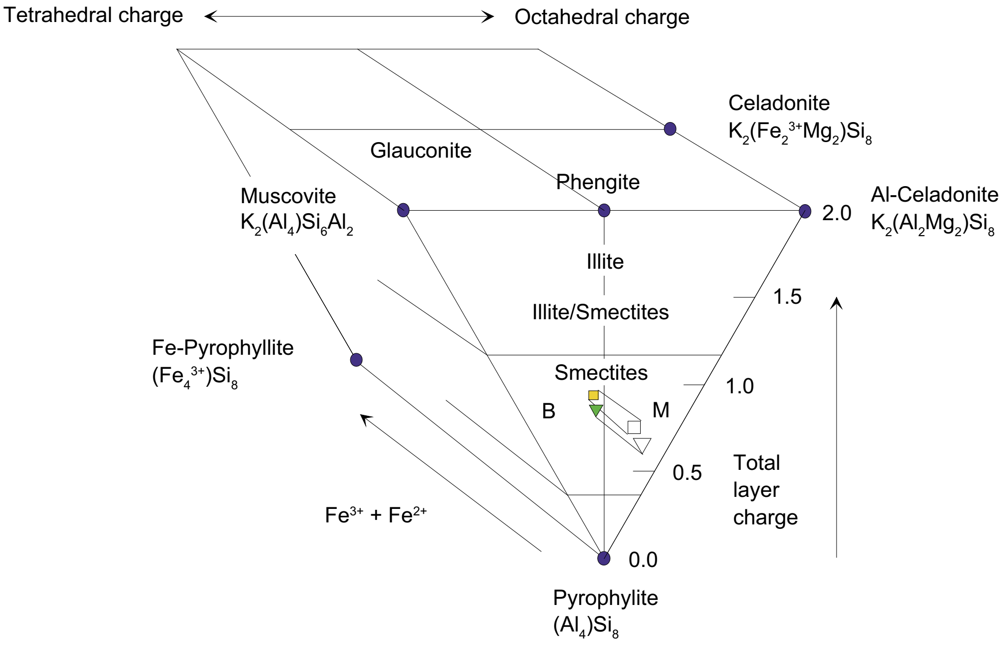

Figure 2-20. *Ideal end-member minerals in the pyrophyllite – mica series with potassium as charge compensating cation, and approximate compositional ranges for illite and smectite (modified from /Newman and Brown 1987/). B denotes beidellite, M denotes montmorillonite. The compositional positions of the montmorillonite minerals in the reference bentonite materials are indicated by a triangle (MX-80) and by a square (Deponite-CAN). All formulas are related to the basic* $O_{20}(OH)_4$ *unit.*

layer smectite-illite) and several models have been suggested in order to describe the reaction. The conversion always involves a charge increase, mainly due to a decrease in silica content and an uptake of charge compensating potassium ions.

Illite material may be illustrated by the mineralogical composition of a natural illite from Montana, US, with less than 10% expandable layers /Hower and Mowatt 1966/:

$(Si_{6.81} Al_{1.19})$	$(Al_{3.25} Fe_{0.14} Mg_{0.59})$	$O_{20} (OH)_4$	$Ca_{0.1} Na_{0.02} K_{1.53}$
tetrahedral	octahedral		interlayer

which can be compared with the composition of the montmorillonite in the MX-80 SR-CAN reference bentonite:

$(Si_{7.86} Al_{0.14})$	$(Al_{3.11} Fe^{3+}_{0.37} Mg_{0.50})$	$O_{20} (OH)_4$	$Na_{0.47} Ca_{0.05} Mg_{0.02} K_{0.01}$
tetrahedral	octahedral		interlayer

The main differences being that the illites have approximately one unit charge higher tetrahedral charge, and potassium as the main charge compensating cations. It is generally accepted that a transformation may take place by release of silica from the montmorillonite tetrahedral sheet, and that no complete dissolution of montmorillonite is necessary. Simplified, the total illitization reaction may be expressed:

Ca^{2+}/Na^{+}-montmorillonite + K^{+} + (Al^{3+}) → Illite + Silica + Ca^{2+}/Na^{+}

In massive natural sediments the physico-chemical conditions are similar over huge volumes, and concentration gradients are generally insignificant. The total reaction therefore involves a series of sub-reactions; release of silica from montmorillonite, release of potassium from e.g. feldspars, potassium fixation and precipitation of new silica minerals, and the total reaction rate is governed by the slowest of the sub-reactions.

According to the equilibrium conditions for 25°C shown in Figure 2-21, the montmorillonite will be thermodynamically stable for silica activities over 1 mM, and silica has to precipitate or be transported away in order to let an illitization reaction take place. Amorphous silica, with an equilibrium activity of around 2 mM, may consequently prevent the dissolution of silica from montmorillonite, but quartz may not. Quartz precipitation may therefore be a kinetically controlling mechanism in illitization of natural montmorillonite sediments /Abercrombie et al. 1994/. The precipitation of quartz may therby lead to a secondary effect of montmorillonite alteration in the form of cementation of the buffer.

Kinetic models have been developed for calculation of degree of transformation in smectite-to-illite transformation. Relationships and constants have been established by means of laboratory batch experiments and comparisons with natural systems /e.g. Eberl and Hower 1976, Pytte 1982, Huang et al. 1993, Cuadros and Linares 1996/. Most models have the form of an Arrhenius expression and the Huang et al. model may be shown as an example:

The overall kinetics of the smectite-to-illite reaction can be described by equation #:

$$-dS/dt = A \cdot [K^+] \cdot S^2 \cdot \exp(-E_a/RT), \qquad (2\text{-}32)$$

where S is the smectite fraction in the illite/smectite material, A is frequency factor, E_a is activation energy and R is the universal gas constant, and T is temperature. After integration of Equation 2-32 the smectite content at a certain time can be calculated if the temperature and potassium concentration in the pore water are known. The potassium concentrations in the Äspö groundwater are measured to be in the range of a few ppm up to 80 ppm /Nilsson 1995/. According to the model, practically no clay conversion is possible in a KBS-3-type repository at these conditions as shown in Figure 2-22.

Brammallite/rectorite may be seen as a sodium equivalent to illite. The mean layer charge is higher than in illite, normally close to 2 units charges per $O_{20}(OH)_4$. Chlorites have the same basic structure as montmorillonite, but the layer charge is normally close to 2 units charges per $O_{20}(OH)_4$. The layer charge is balanced by positively charged, octahedrally coordinated, hydroxide sheets. The central ion in the interlayer hydroxide sheet may be any di- or tri-valent metal ion, normally Mg, Al or Fe. Transformation of montmorillonite into brammallite/rectorite and chlorites are theoretically possible if potassium is not available, and release of silica from the montmorillonite continues until the required tetrahedral charge is reached. Both brammallite/rectorite and chlorites are less commonly found as alteration products of montmorillonite in natural sediments compared to illites.

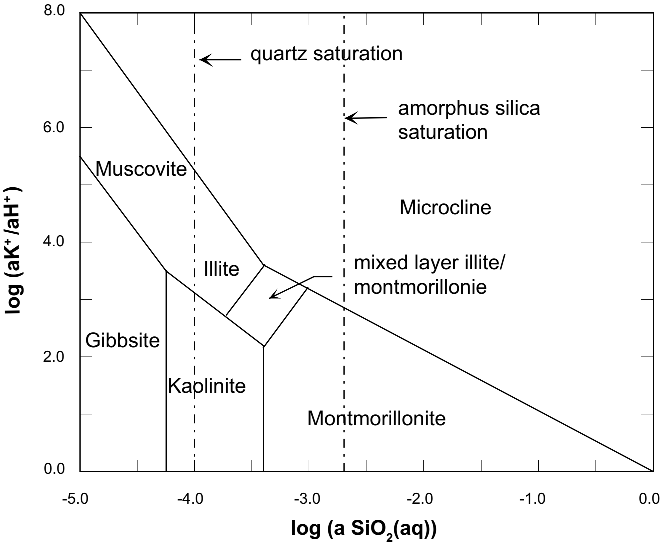

Figure 2-21. *Silica mineral equilibria with the partial component potassium at 25°C. (Simplified from /Aagard and Helgeson 1983/).*

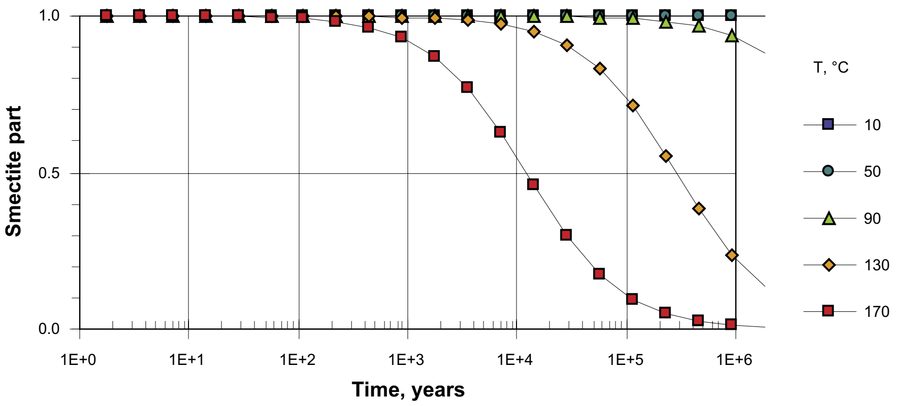

***Figure 2-22.** Remaining smectite part for different temperatures in a hydrothermal system with [K^+] = 0.002 mole/litre (80 ppm) according to the Huang et al. kinetic model and laboratory determined constants (E_a = 27.4 kcal/mole and A = 8.5E4) /Karnland 1995/. Legend shows temperature in °C.*

Transformation due to iron reactions

The octahedral layer in montmorillonite frequently contains a significant amount of iron which may change oxidation state /Stucki et al. 1984/. Normally, the iron is in an oxidized condition in commercial material due to exposure to air during mining and handling. Reduction to Fe(II) would lead to an increase of the total layer charge, and a potential fixation of interlayer cations if the charge change is sufficient. The effect of such octahedral layer change is expected to have less effect compared to a similar charge change in the tetrahedral layer /Spositio 1999/. The SR-Can reference bentonites contain 0.37 Fe (MX-80) and 0.45 Fe (Deponit CA-N) per $O_{20}(OH)_4$ unit /Karnland and Birgersson 2006/.

Dissolution of silica due to high pH

The groundwater pH may be significantly increased by use of cement materials in the repository. The solubility of silica minerals increases strongly with increasing pH, see Figure 2-23, which consequently may lead to dissolution of tetrahedral silica in montmorillonite, general dissolution of montmorillonite, and a parallel dissolution of other silica minerals. If a pH gradient prevails in the system the resulting activity gradient will lead to significant transport of dissolved silica, and a charge change in the tetrahedral layer in the montmorillonite. Precipitation of new silica minerals may lead to the same silica depletion in the montmorillonite in both stagnant high pH conditions and in pH gradient conditions,

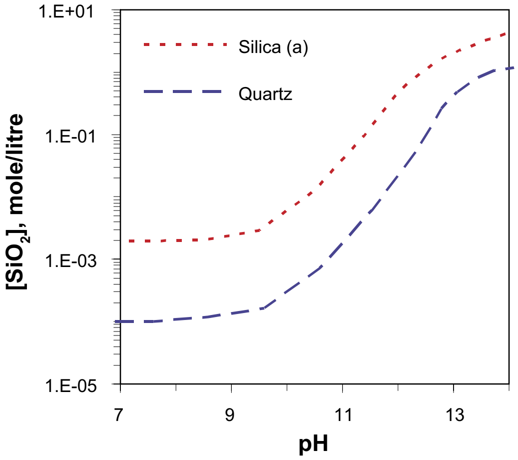

***Figure 2-23.** Silica equilibrium activity conditions for amorphous silica and quartz versus pH as calculated by PHREEQC/Lawrence Livermore database.*

Effects of transformation

Change in the layer charge of the montmorillonite leads to change in the interaction with water and thereby to effects on the swelling pressure. On illitization and similar alterations the interaction virtually ceases and the water previously bound between the individual layers is released. The pore geometry is thereby changed towards fewer and larger pores. Swelling between remaining montmorillonite layers will partially counteract the pore increase, and the quantity of remaining montmorillonite will thereby determine the system's swelling pressure and hydraulic conductivity. The sensitivity to the ion content of the pore water increases with the degree of transformation, and released silicon is expected to lead to a deterioration of the buffer's rheological properties due to precipitation in the pore volume. A total transformation of all the montmorillonite in the buffer into illite or similar minerals would lead to complete loss of buffer functions.

Table 2-17 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Boundary conditions

The relevant boundary conditions in order to treat the process quantitatively are the absolute temperature and the temperature gradient, and the transport processes that control the exchange of solutes between the buffer pore water and the water in its adjacent components, i.e. the boundary conditions of the processes diffusion and advection.

Table 2-17. Process/variable table for the process Montmorillonite transformation.

Variable	Does this variable influence the process?		Does the process influence this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Buffer geometry	Amount of buffer	Included in evalutaion	At extreme tranformation	–
Pore geometry	Indirect through Bentonite composition		Indirect through Bentonite composition	
Radiation intensity	No		No	
Temperature	Yes	Included in transformation expression	No	
Water content	Reduced transformation in unsaturated clay	No credit taken	At extreme tranformation	
Gas content	No		No	
Hydrovariables (pressure and flows)	Supply of water (potentially harmful species)	Included in transformation evaluation	Indirect through Bentonite composition	Effect on hydraulic conductivity is evaluated
Stress state	No		Yes	Loss of swelling is evaluated
Bentonite composition	Yes	Included in transformation expression	Yes	Included in transformation expression
Montmorillonite composition	Yes	Included in transformation expression	Yes	Included in transformation expression
Pore water composition	Harmful species	Included in transformation expression	(Yes) to a small extent	Only effects on the buffer itself are considered
Structural and stray materials	Amount and type of cement	Assumed “safe” in SR-Can	No	

Model studies/experimental studies

The illitization process is of great importance from several viewpoints in connection with prospecting and extraction of oil deposits. The great commercial interest, in combination with the mineralogically interesting process, has led to very extensive research since the 1960s. A large number of publications therefore exist as a basis for the assumption that the transformation processes is not expected to be important in a deep repository. The argumentation can be summarized in three points:

1. The bentonite material is close to mineralogical equilibrium to start with /e.g. Fritz et al. 1984/.
2. Temperature-induced transformation is limited by a shortage of K^+ /Hökmark 1995/.
3. The transformation rate at the repository's maximum temperature is very low /e.g. Eberl and Hower 1976, Pytte 1982, Huang et al. 1993/.

The mineralogical stability is studied in the Lot tests at Äspö HRL. The test conditions represent repository conditions, and adverse conditions in order to accelerate possible degradation processes. The adverse conditions involve:

- Higher temperature.
- Higher temperature gradient.
- Higher content of accessory minerals (calcite, gypsum, K-feldspar).
- Introduction of new substances (Portland cement).

In the 5-year tests, only the effect of increased temperature in the "adverse condition tests" will simulate the major period of elevated temperature in a KBS-3 repository, with respect to kinetically governed processes. The introduction of additional substances and increased temperature gradients is made in order to accelerate also processes, which are governed by transport of substances. The effect of the temperature gradient is, however, not possible to describe in an as simple and general way as the effect of increased temperature and concentrations of reactants.

Natural analogues/observations in nature

Besides in SKB-related investigations, the transformation of smectite to illite is well-documented for a large number of geological formations. Natural sediments have been studied by, among others, /Burst 1959, Perry and Hower 1970, Hower et al. 1976, Colten-Bradley 1987, Lynch 1997/. The studies show that increased sediment depth (increasing temperature) leads to increased illite content, and that low availability of potassium can be linked to reduced transformation. Silica activity as kinetically controlling factor has been studied in sediments /Abercrombie et al. 1994/. Special formations where temperature effects have been obtained from e.g. volcanic activity have revealed a similar transformation /e.g. Pytte 1982, Lynch 1985, Brusewitz 1986/. Cementation effects as a consequence of transformation have been studied specifically by, among others, /Hower et al. 1976, Boles and Franks 1979/.

Time perspective

Precipitation and montmorillonite layer charge changes may take place during the initial temperature gradient phase. Significant changes in the montmorillonite content of the buffer are expected to occur on a million-year timescale according to illitization models.

Handling in the safety assessment SR-Can

Different conditions in the repository evolution may alter the composition of the buffer. The most important may be an elevated temperature or an intrusion of an alkaline solution:

Temperature:

Model: The maximum temperature effect will be modelled by the kinetic expression proposed by Huang et al. for illitization for different realistic concentrations of potassium. The temperature gradient conditions will be modelled by an equilibrium/transport code (PHREEQC) with respect to silica for different interaction with groundwater. The maximum possible transport of silica may be used to quantify the maximum charge effect on montmorillonite, and thereby on all transformation processes except dissolution/precipitation reactions, which is covered by the kinetic model. Full water saturation is assumed in the modelling.

Boundary conditions: The temperature and the composition of the groundwater.

Handling of variables influencing this process: See Model above

Handling of variables influenced by the process: The amount of remaining montmorillonite as a function of time will be calculated. The content of silica impurities will also be calculated.

pH:

Model: The effect of high pH will be modelled by a reactive transport code. The maximum release of silica from montmorillonite may be used to quantify the transformation.

Boundary conditions: Temperature and groundwater composition.

Handling of variables influencing this process: See Model above

Handling of variables influenced by the process: The amount of remaining montmorillonite as a function of time will be calculated. The content of silica impurities will also be calculated.

Uncertainties

Uncertainties in mechanistic understanding

There is a generally accepted explanation to the diagenesis in which smectite is converted into illite accompanied by a release of silica, water and cations. There is, however, no general consensus concerning the details in the smectite-to-illite transformation mechanisms in a repository environment and a number of explanations of the character and mechanisms of the smectite-to-illite conversion have been proposed /Moore and Reynolds 1989/:

Model simplification uncertainties for the above handling in SR-Can

Laboratory experiments have shown transformation rates, which are faster than predicted by the kinetic models under the following extreme conditions, which consequently are not covered by the present models:

- Low water content influence /Couture 1985/.
- Repeated drying-out, /Karnland et al. 1994/.
- pH effects /high pH: Velde and Vasseur 1992/, /Savage et al. 2002/, /Gaucher et al. 2004/, /Karnland et al. 2005b/; low pH: /Zysset 1992/.

Input data and data uncertainties for the above handling in SR-Can

Thermodynamic and kinetic data for modeling silica dissolution/precipitation are not well known especially for high pH and high temperatures. In transport calculations, the diffusion constants in rock and bentonite constitute an uncertainty. For obvious reasons, the kinetic model constants are determined in laboratory experiments performed with relatively short duration time and at high temperatures and high potassium concentrations compared to the natural conditions it is aimed to describe. The various illitization models currently available show a large variety in constant values and model formulas, which indicates conceptual problems.

However, the set of determined constants and formulas generally results in similar long-term predictions /Karnland and Birgersson 2006/.

2.5.10 Montmorillonite colloid release

Overview/general description

The uptake of water and resulting swelling of the bentonite buffer is counteracted by the walls of the deposition hole, and a swelling pressure is developed in the bentonite (see Section 2.4.1). Fractures intersecting the deposition hole mean that rigid swelling restrictions are not present everywhere, and that localized swelling continues into the fractures until a thermodynamic equilibrium is reached without the development of swelling pressure. This free swelling may lead to separation of individual montmorillonite layers, or small groups of mineral layers (dispersion). This means that part of the buffer could enter the aqueous phase and be transported with the groundwater.

The maximum free swelling is strongly dependant on the salinity of the groundwater. The interlayer distance may be discussed in terms of the Debey-Hückel screening length theory, which predicts a spacing change inversely proportional to the square root of solution concentration, which has been experimentally confirmed.

At low concentration the distance between the individual montmorillonite layers may be large enough to let the clay particles be dominated by thermal motion i.e. they have colloidal properties. The individual colloidal particles may then be transported away from the deposition hole in fractures by diffusion or by groundwater flow in the fracture.

In general, the stability of such a colloidal system can ideally be evaluated from DLVO theory (central theory in surface chemistry) in which all attractive and repulsive forces between individual montmorillonite layers are taken into account. Coagulation of a dispersed system may be achieved by adding an electrolyte, and the higher the valence, the more efficient is the coagulation. A critical coagulation concentration (CCC) may be determined for different solutions, and this CCC-value may be used as a conservative value for preventing swelling to an extent where montmorillonite will appear as a colloid.

The critical coagulation concentration (CCC) may be determined for different solutions, and used as a conservative value for spontaneous colloid formation. Groundwater concentration has to be at least 0.1 M with respect to sodium (monovalent) ions or 0.001 M calcium ions (divalent ions) in order to neglect colloid formation. If this is not achieved mass transport modelling, including diffusive and flow transport, has to be made.

The following table summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can. Note though that the process occurs at the boundary between buffer and rock, within rock fractures making the boundary conditions described below of prime importance for the understanding and quantification of the process.

Boundary conditions

The boundary conditions are the cation concentration and cation valency of the groundwater in direct contact with the outermost part of the bentonite buffer.

Water flow in the fractures will not affect the stability of true colloids. However, the interlayer distance between the montmorillonite layers is continuously increasing with decreasing electrolyte concentration and layers at large separation are more sensitive to erosion than layers at close separation. Water-flow may consequently tear loose mont-morillonite layers although the distances are shorter than what is needed for true colloids. The extent of such particle formation by flow is consequently dependent on the flow velocity, and the particles are not stable without flow. The treatment of erosion is presented in Section 2.3.4.

Table 2-18. Process/variable table for the process Montmorillonite colloid release.

Variable	Does this variable influence the process?		Does the process influence this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Buffer geometry	Amount of buffer present	Included in evaluation	Buffer loss	Included in evaluation
Pore geometry	No		No	
Radiation intensity	No		No	
Temperature	Negligible		No	
Water content	Indirect through stress state		No	
Gas content	No		No	
Hydrovariables (pressure and flows)	May determine the rate of colloid release	Included in current model	Indirect through buffer geometry	
Stress state	Yes		Indirect through buffer geometry	
Bentonite composition	Impurities may buffer the effect	Included in current model – to a certain extent – not fully understood	(Selective loss of the clay component)	
Montmorillonite composition	Na-montmorillonite more prone to the process than Ca-montmorrillonite	Na-montmorillonite assumed – Not fully understood	No	
Pore water composition	Only occurs if [M2+] < 0.001 M		Colloid source	Only effects on the buffer itself are considered
Structural and stray materials	No		No	

Model studies/experimental studies

The principles for swelling of montmorillonite in electrolyte solutions have been reported in a large number of publications. The basic theoretical principles are described by the DLVO theory /Verwey et al. 1948, Derjaguin and Landau 1941/. Interlayer distances were experimentally determined in by /Norrish and Quirk 1954/, and several subsequent studies have in principle confirmed these results. Several laboratory studies have been made in order to determine the critical coagulation concentration for montmorillonite in sodium and calcium chloride solutions /van Olphen 1963, Le Bell 1978, Wold 2003/.

Natural analogues/observations in nature

In principle, a large number of analyses of Swedish groundwater may serve as natural analogs since they show low contents of clay colloids despite the fact that swelling clay is often found in fractures. Specific studies have been made at the Äspö HRL /Laaksoharju 2003/ and at Grimsel HRL /Degueldre et al. 1996/.

Time perspective

Colloid formation is only relevant at low ion concentrations and likely only relevant in conjunction with a glaciation. The effects may be significant only in the long-term perspective.

Handling in the safety assessment SR-Can

The process is neglected if the sum total concentration of divalent cations exceeds 1 mM. If this condition is not fulfilled, loss due to erosion will be quantified.

To estimate possible losses of buffer mass for glacial conditions, three stylised cases have been simulated. One concerns flow conditions that are similar to those at present and the other two analyse conditions of increased flow. For all these, the buffer pore water is assumed to be depleted of Ca^{2+} ions. This means that Ca^{2+} ions for the prevention of colloid formation will not be supplied by the buffer. Since the groundwater is also depleted in Ca^{2+} ions, the erosion is assumed to occur at a rate that is determined by the product of the equivalent flow rate at the deposition hole and the maximum concentration of bentonite in a water suspension (50 g/L). This model maximises the loss rate assuming that the mass exchange between the bentonite suspension and the flowing water is driven by diffusion. However, mechanistic understanding of the colloid release process is insufficient for robust estimation of erosion. For example, the repulsive forces between the clay particles are not considered in the model used, and these forces act to increase the loss rate. The model also assumes that the bentonite consist of only montmorillonite which is converted to a pure Na-form. There are early experimental and theoretical indications that the extent of the colloid release process could be much smaller in the case of a commercial bentonite and especially a bentonite with calcium as the dominant cation. This means that further knowledge may lead to models that yield both lower and higher loss rates.

Uncertainties

Uncertainties in mechanistic understanding

The knowledge concerning colloid formation and colloid stability is good concerning the effects of mono- and di-valent ions. The effect of trivalent ions is theoretically significantly larger than for divalent ion and could possibly serve as a less conservative criterion. The effects are not well established in laboratory experiments for the actual conditions. The possible transport of colloids by diffusive and flow transport is less well known. The effects of mechanical erosion of loose gels close to colloid conditions have not been examined.

Model simplification uncertainties for the above handling in SR-Can

The suggested treatment in SR-Can is based on a simplified, scoping model. It should be noted that a number of simplifying assumptions have been made.

The following assumptions must be revisited and checked for reasonableness

1. The change of composition in the diffuse layer is not accounted for.
2. Steady state assumption for clay intrusion into the fracture.
3. Steady state assumption of the chemical transport.
4. Applicability of Q_{eq} model.
5. Assumption of no mechanical erosion of gel fringe.
6. Assumption of Ca mineral dissolution.
7. Assumption of steady-state for chemistry e.g. no pH changes that influence the CCC.

The above items can all conceivably influence (increase) the dispersion rate. There may be more that will be found in a more detailed investigation

The following could act to decrease the dispersion rate

1. The diffusion resistance in the clay in the fracture is neglected.
2. The change of composition in the diffuse layer is not accounted for.

3. Physical hindering of clay particle dispersion in the fracture.
4. Clogging of water pathways by the clay being pressed out into the fracture.
5. Sedimentation of clay particles in fracture.
6. Development of a montmorillonite depleted region near the fracture entrance leaving behind sparsely soluble minerals that "clog" the fracture entrance.

There may be more effects that will be found in a more detailed investigation

Input data and data uncertainties for the above handling in SR-Can

The evolution of groundwater composition, and groundwater flow conditions are the important uncertainties. These will be evaluated in integrated assessment modellings, see further the Interim report of the safety assessment SR-Can.

2.5.11 Radiation-induced transformations

Overview/general description

Montmorillonite in the buffer can be broken down by γ radiation. The result is a decrease in the montmorillonite concentration.

In the case of a failed canister, radionuclides sorbed in the buffer could possibly affect the properties by α radiation.

Table 2-19 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Table 2-19. Process/variable table for the process Radiation-induced transformations.

Variable	Does this variable influence the process?		Does the process influence this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Buffer geometry	No		No	
Pore geometry	No		No	
Radiation intensity	Yes	Dose rates are too low to cause any significant transformations – the process is excluded from SR-Can	No	
Temperature	No		No	
Water content	No		No	
Gas content	No		No	
Hydrovariables (pressure and flows)	No		No	
Stress state	No		No	
Bentonite composition	?	Not detected	(Yes)	Dose rates are too low to cause any significant transformations – the process is excluded from SR-Can
Montmorillonite composition	?	Not detected	No	
Pore water composition	No		No	
Structural and stray materials	No		No	

Boundary conditions

A quantitative treatment of the process requires knowledge of the radiation field in the buffer, which is obtained from the process Radiation attenuation, Section 2.1.1.

Model studies/experimental studies

Experimental studies have shown that the accumulated radiation doses to which the bentonite will be exposed in a deep repository do not cause any measurable changes in the montmorillonite concentration. MX-80 bentonite saturated with weakly brackish water to a density of 2,050 kg/m^3 was irradiated for one year with a total radiation dose of $3 \cdot 10^7$ Gy, which is orders of magnitude more than what will be the case in the repository. The specimen was confined in a cylinder whose one closed end consisted of iron and irradiated with a ^{60}Co source, while the other end consisted of a porous steel filter through which a water pressure of 1.5 MPa acted /Pusch et al. 1993/. The irradiated end, which had an absorbed dose rate of 3,972 Gy/h, was kept at 130°C, and the opposite end, which had a dose rate of 456 Gy/h, at 90°C. Mineral assays (XRD, IR, CEC) of this specimen and of a parallel specimen not exposed to radiation but to the same hydrothermal environment as the irradiated specimen, showed no significant change in the montmorillonite quantity in either of the specimens.

In /Andersson 1984/ it is shown that an α-dose of $4 \cdot 10^{18}$ alphas/g bentonite will totally destroy the material. In the RN-caculations for SR 97 it was found that the total concentration of α-emitters in the buffer closest to the canister would give a total dose of $8 \cdot 10^{15}$ alphas/g of bentonite for the first million years with the assumption of an early canister failure (this is less than 1% of the dose required to destroy the material closest to this canister). In most parts of the buffer the the α-dose will much less since the α-emitters are stongly sorbed and will stay in the vincinty to the canister. This means that on a very small part of the buffer will be affected and then not likely substantially.

Natural analogues/observations in nature

Not applicable.

Time perspective

See Section 2.1.1.

Handling in the safety assessment SR-Can

Based on the experimental and modelling studies mentioned above it is shown that the effect of radiation on buffer properties is insignificant and the process is therefore neglected.

Uncertainties

There are no uncertainties of relevance to the safety assessment.

2.5.12 Radiolysis of pore water

Overview/general description

Gamma radiation from the fuel that penetrates through the canister can decompose pore water by radiolysis, forming OH radicals, H_2, O_2 and several other components. The oxygen is consumed rapidly by oxidation processes that affect the redox potential, while the hydrogen may be transported away. The canister's wall thickness is, however, sufficient so that the effect of γ-radiolysis on the outside is negligible /Werme 1998/.

The following table summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Process/variable table for the process.

Boundary conditions

A quantitative treatment of the process requires knowledge of the radiation field in the buffer, which is obtained from the process Radiation attenuation.

Model studies/experimental studies

Corrosion of copper in water in the presence of γ-radiation has been studied in a few experiments. These are summarized in /King et al. 2001/. The results show no effect on the corrosion rate even with higher dose than those expected in the repository.

Natural analogues/observations in nature

Not applicable.

Time perspective

The γ radiation is significant during the period approximately 1,000 years following canister installation.

Table 2-20. Process/variable table for the process Radiolysis of pore water.

Variable	Does this variable influence the process? Influence present?	Handling of influence?	Does the process influence this variable? Influence present?	Handling of influence?
Buffer geometry	(Yes)		No	
Pore geometry	No		No	
Radiation intensity	Yes	Dose rates are too low to cause any significant radiolysis outside canister – the process is excluded from SR-Can	No	
Temperature	No		No	
Water content	Yes		No	
Gas content	(Yes)		No	
Hydrovariables (pressure and flows)	No		No	
Stress state	No		No	
Bentonite composition	No		No	
Montmorillonite composition	No		No	
Pore water composition	Yes	Dose rates are too low to cause any significant radiolysis outside canister – the process is excluded from SR-Can	Yes	Dose rates are too low to cause any significant radiolysis outside canister – the process is excluded from SR-Can
Structural and stray materials	No		No	

Handling in the safety assessment SR-Can

Radiolysis of the porewater could potentially increase the corrosion rate of the copper canister. However, the experiments mentioned above clearly show that the consequences of radiolysis are very limited. The process is therefore neglected in SR-can

Uncertainties

There are no uncertainties currently identified that are of relevance to the safety assessment.

2.5.13 Microbial processes

Overview/general description

Microbial processes can under certain conditions result in the formation of gas and sulphide /Pedersen 2002/. Gas formation can give rise to disrupting mechanical effects on the buffer, and sulphide from sulphate reducing bacteria (SRB) can corrode the copper canister. Sulphide formation must take place in the buffer, near the canister, and be of considerable extent for corrosion to be a threat to the canister integrity, mainly due to the fact that the solubility of sulphide, and thereby its diffusive transport capacity, is very low. In order for the above-described processes to take place, the bacteria must be active and have access to water, nutrients and space /Pedersen 2002/.

Sulphate reducing bacteria are very common in deep Fennoscandian groundwater. They are reported to occur abundantly down to depths of at least 600 to 700 m /Haveman and Pedersen 2002, Pedersen et al. 2000b/. Microbes are generally very robust and can withstand harsh conditions. The potential for sulphide production is significant at repository depth and possible effects on the repository function must be considered in safety assessment.

Table 2-21 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Buffer geometry: The volume of the buffer is not important for this process

Pore geometry: Pores with sizes smaller than about 200 nm can not be penetrated or inhabited by microbes. Microbes vary in size from about 200 nm up to 600 µm.

Radiation intensity: Microbes are generally radiation resistant, but it varies from species to species. Increasing dose will decrease the number of surviving microbes.

Temperature: All microbes have a temperature range within which they are active. Increasing the temperature will increase microbial activity. Temperatures above the maximum are lethal. Highest know temperature for microbial life is about 110–120°.

Water content: Decreasing water availability reduces the diversity. Many microbes can compensate a low water content using metabolic, energy consuming processes. Water is needed for active life. A combination of low energy availability and low water content is detrimental to many microbes.

Gas content: Hydrogen and methane can be consumed by microbes; largest effect is obtained if oxygen is present. Active microbes can produce gas if organic carbon is available for metabolism.

Hydrovariables (pressure and flows): Most microbes tolerate large variations in hydrostatic pressure and flow.

Stress state: Microbes tolerate limited mechanical pressure. Swelling clay will disrupt microbes when the pore size becomes smaller than the size of the microbe.

Table 2-21. Process/variable table for the process Microbial processes.

Variable	Does this variable influence the process?		Does the process influence this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Buffer geometry	No		No	
Pore geometry	Yes	No microbial activity assumed for buffer densities over 1,800 kg/m^3	No	
Radiation intensity	Yes	No credit is taken for the radiation field	No	
Temperature	Yes	The effect of temperature is neglected. If at all, microbial effects will be important after the thermal period	No	
Water content	Yes	No credit is taken for a partially saturated buffer.	No	
Gas content	Yes	The effect of hydrogen and methane is considered.	Yes	Only effects on the buffer/canister are considered
Hydrovariables (pressure and flows)	(No)		No	
Stress state	Yes	No microbial activity assumed for buffer densities over 1,800 kg/m^3	No	
Bentonite composition	Yes	Neglected since the amount of organic carbon in the buffer is limited	No	
Montmorillonite composition	(No)	Nothing known	No	
Pore water composition	Yes	Determines the corrosion rate. Included for the case where the buffer density is below 1,800 kg/m^3	(Yes)	Only effects on the buffer/canister are considered
Structural and stray materials	Yes	Not considered within SR-Can	Yes	Not considered within SR-Can

Bentonite composition: There is a positive correlation between microbial activity and the concentration of organic carbon.

Montmorillonite composition: Nothing known

Pore water composition: There is a positive correlation between microbial activity and the concentration of organic carbon. There is a limited effect on the pore water chemistry if the microbes are metabolically active. Gas and sulphide production can theoretically occur.

Structural and stray materials: There is a positive correlation between microbial activity and organic carbon present in stray material. Microbial degradation of organic stray material is possible.

Boundary conditions

There are no particular boundary conditions to discuss for this process. The relevant boundary conditions in order to treat the process quantitatively are those of the transport processes that control the exchange of solutes (microbe nutrients) between the buffer pore water and the water in its adjacent components, i.e. the boundary conditions of the processes diffusion and advection.

Model studies/experimental studies

A Large scale Canadian buffer experiment

A full-scale experiment (Buffer-Container Experiment, BCE), with buffer material consisting of 50/50% bentonite/sand was performed at Atomic Energy of Canada Limited´s (AECL) underground laboratory in Canada. The results showed that microbes, with a few exceptions, could only be cultured from buffer samples with a gravimetric water content of 15% or more, which is approximately equivalent to the water content in a 100% bentonite having a saturated density of 2,000 kg/m^3 /Stroes-Gascoyne et al. 1997/. Elevated temperatures had no effect on the microbes. These results were interpreted as an effect of limited availability of water. The result of the BCEraised questions about the survival of microbes, and especially SRB, in buffer materials in 100% bentonite and has subsequently led to detailed laboratory experiments.

Laboratory experiments exploring the survival of bacteria in buffer

The Canadian field experiment was followed up by laboratory experiments. Two species of sulfate reducing bacteria were mixed with MX-80 bentonite at varying densities, from 1,500 kg/m^3 to 2,000 kg/m^3 /Motamedi et al. 1996/. The species were *Desulfovibrio aespoeensis* and *Desulfomicrobium baculatum*, both isolated from deep groundwater at the Äspö HRL. None of the species survived 60 days at densities above 1,800 kg/m^3. *D. baculatum* survived the better of the two, remaining culturable for 60 days at 1,500 kg/m^3. Although microbial activity rapidly diminished, it was argued that this was due to the laboratory conditions during this experiment, which may have added some extra constraints to the ones found in the field situation. The laboratory experiment represents a closed situation with an artificial microbial population, while field conditions would be of the open system type with a natural microbial population. A long-term field experiment was therefore initiated to assess microbial issues.

Survival of microbes in long term buffer tests with in situ conditions

The long-term test (LOT) of buffer performance aims to study models and hypotheses of the physical properties of a bentonite buffer. Several species of bacteria with different relevant characteristics were introduced into the LOT bentonite. Mesophilic, thermophilic and spore-forming sulfate reducing bacteria, together with desiccation resistant, chemo-organotrophic or chemolithotrophic spore- and non-spore forming bacteria were mixed with bentonite clay to give approximately 100 million bacteria per gram (dry weight) of clay /Pedersen et al. 2000a/. The clay with bacteria was subsequently formed into cylindrical plugs with a 20 mm length and diameter, and installed in bentonite blocks exposed to low (20–30°C) and high (50–70°C) temperatures. The blocks were installed in the LOT boreholes immediately after the bacteria plugs were introduced /Pedersen et al. 2000a/. The experiment was terminated after 15 months. The major outcome was the effective elimination, to below detection limits, of all bacteria except the spore-forming ones. All of the three spore formers survived at the low temperature. The numbers remaining were, however, much lower than those initially introduced. The approximately 100 million spore-forming bacteria per gram (dry weight) of clay were reduced 100- to 10 000-fold. This can be interpreted as showing that the cell death rate was higher than the growth rate, which may have been zero, or close to zero. The spore-forming sulfate reducing bacterium was the only one of the three that survived at high temperature. It was concluded that the spore formers most probably survived as spores, and spores do not produce sulphide.

Survival is not equivalent to activity. Since the methods used in this experiment did not reveal activity, additional experiments were set up to include measurement of sulphide production in simulated repository conditions.

Laboratory experiments exploring microbial sulphide production in buffer

The worst-case scenario in copper canister corrosion would be if SRB formed biofilms on the canisters or grew intensively in the buffer close to the canister. To mimic this situation, several experiments have been executed and evaluated. In a first series, swelling pressure oedometers were loaded with bentonite at different densities, corresponding to different water activity values /Pedersen et al. 2000b/. A copper disc was placed between the bottom lid and compacted bentonite. Different SRB were added to the clay and the discs, together with $^{35}SO_4^{2-}$. The species used were laboratory cultures. Finally, oxidised silver foil was placed between the disc and the clay. The oedometers were reassembled and incubated for 4 weeks at the respective optimum temperatures and three different saturated densities: 1,500, 1,800 and 2,000 kg bentonite/m^3, corresponding to the water activities 0.999, 0.994, and 0.964, respectively. After incubation, $^{35}S\text{-}Ag_2S$ was localised on the silver foils and quantified by electronic autoradiographic imaging (Packard instant imager electronic autoradiography system, Meriden, U.S.A.). The amount of Ag_2S formed was used as a measure of the sulphate reducing activity.

The SRB used were active at a bentonite density of 1,500 kg/m^3, but that sulphide production was virtually absent at higher densities. This experiment indicated that SRB probably cannot be active at the canister surface at a repository density of 2,000 kg/m^3. However, the experiment was run with two laboratory species and it may be possible that other species that were not tested could survive better. Therefore, additional experiments were carried out using natural groundwater that commonly contains many hundreds of different microbial species, including several naturally occurring species of SRB.

Field experiments exploring microbial copper sulphide production in buffer

The activity of SRB was again investigated in compacted bentonite with densities of 1,500, 1,800 and 2,000 kg/m^3 using stainless steel oedometers with $^{35}SO_4^{2-}$ as an oxidized sulphur source for the SRB respiratory processes /Masurat and Pedersen 2003/. This time, the investigations were performed under in situ conditions, including a hydrostatic pressure of 25 bars at a depth of 450 m at the Äspö Hard Rock Laboratory. The sources of SRB were the groundwater and the bentonite. Cultured SRB were not added. Canister type copper plates were placed in the oedometers, with the top either in contact with the added groundwater (exposed) or with 3–4 mm bentonite between the plate and the added groundwater (embedded). The initial slot between bentonite and rock in a repository was simulated by a gap between the water inlet filter and the compacted bentonite. The bentonite density was thereby initially low at this end of the sample. The water uptake into the sample led to a density homogenization and a successive increase of density to the final test density. Radioactive hydrogen sulphide formed by the SRB reacted with the copper and formed radioactive copper sulphide, which was measured by electronic radiography as described for the lab experiments above. A similar set-up with filter-sterilized groundwater (0.2 µm) was used as control. Finally, a third bentonite set-up was heat treated at 120°C for 12 h and added with sterile groundwater. The results showed that SRB were active and produced hydrogen sulphide during the initial phase of bentonite swelling, which was monitored for about 70 days. The copper sulphide production by the SRB was inversely related with the final density of the bentonite as the highest density had the lowest overall SRB activity (Figure 2-24).

The experiments with sterile groundwater and sterile groundwater and heat treatment of the bentonite showed that SRB were present in a dormant state in the commercial MX-80 bentonite. By addition of water, these dormant SRB became active and started to produce hydrogen sulphide. It is obvious that the sources of SRB to buffer material are two; the groundwater and the bentonite itself.

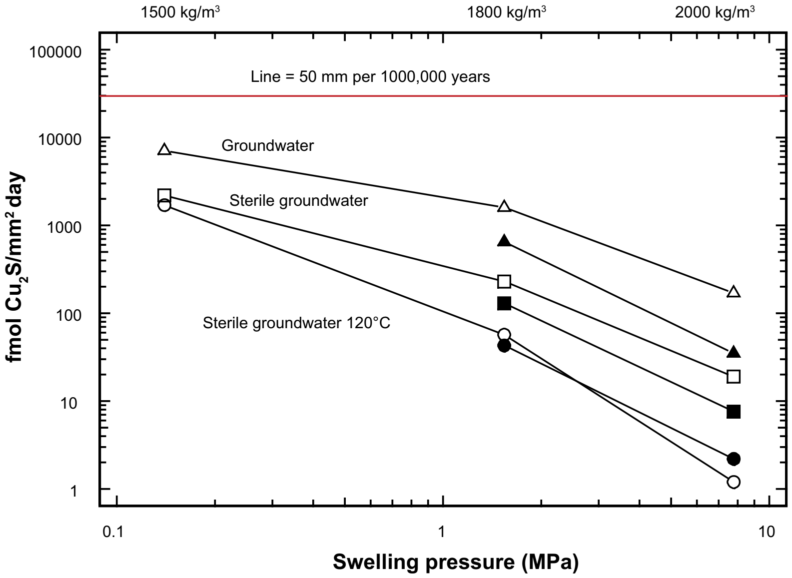

Figure 2-24. *Microbial copper corrosion rates under field conditions with natural groundwater populations from 450 m as function of swelling pressure and experimental configuration. Open symbols show exposed copper plates. Solid symbols show embedded copper plates. The red line indicates the copper sulphide production rate needed to fully corrode a canister in 1 million years.*

Natural analogues/observations in nature

There is a natural analogue in Dunarobba, Italy, where a bentonite slide buried a forest approximately one and a half million years ago. Trees that have not been decomposed by microorganisms can still be found. This indicates that conditions for microbial activity in bentonite clay are unfavourable.

Time perspective

The time perspective concerning survival and activity of microbes in compacted bentonite has been summarized in a conceptual model as follows /confer Figure 3-4 in Pedersen 2000c/. At the time of deposition, there will be a canister, bentonite blocks and a hole in the rock. The next step will be to allow water to fill up all the void volume. This water can be groundwater from the rock or, alternatively, groundwater or technical water added from above at the time of container deposition. Irrespective of the source, microbes will be present in the water and these microbes will mix with the buffer, as described above.

The swelling of the clay will introduce groundwater microbes into the clay, to a depth that is dependant on the initial slot, on both the rock and the canister side of the bentonite, and the microbes indigenous to the bentonite will be present in the entire bentonite buffer. The experimental data on survival and activity of microbes in bentonite suggest that the number of viable microbes will decrease rapidly during swelling and that very few viable cells will be present at full compaction. Sulphate reducing activity will also approach zero when full compaction is achieved and the only survivors will be microbes that have formed spores. Our results indicate that viable cell activity will be impossible at full compaction, as spores are inactive. Although spores generally are very resistant to difficult environmental conditions, they do still die off. All our experiments so far indicate a decrease in the number of viable spores at full compaction so that a slow but significant death rate of spores would eventually lead to the complete eradication of life in the buffer. It has not yet been clarified whether this will occur in the lifetime of a radioactive repository. Once the bentonite becomes sterile, it will most probably not be re-infected. The theoretical pore size of the clay is 100–1,000 times smaller than the average-sized microbe, meaning that no new microbes can enter into the buffer.

Handling in the safety assessment SR-Can

There is a limit to the rate of microbial sulphide corrosion that must not be exceeded. This rate is defined by the thickness of the canister and is based on the assumption that sulphide corrosion of copper is of a non-pitting type. A production rate of about 25 pmol Cu_2S/mm^2 and day will corrode 50 mm depth of a canister in 1 million years (Figure 2-24). If the safety limit is set to 0.25 pmol Cu_2S/mm^2 and day, the corrosion will correspond to 0.5 mm over 1 million years, leaving 49.5 mm of the canister intact. This safety limit corresponds to the maximum measured initial corrosion rate at a swelling pressure of about 8 MPa (2,000 ton/m^3) under field conditions (Figure 2-24). Decreasing swelling pressure will result in an increasing microbial copper sulphide production rate. The microbial copper sulphide production rate also depends on the diffusion rate of nutrients and sulphide, radiation intensity, the water content and the level of heat stress.

Microorganisms are expected to be eliminated in the bentonite due to the sum of several severe stress factors present during the initial centuries. Once gone, the low pore size is expected to hinder re-colonization with concomitant sulphide and/or gas formation.

Uncertainties

Uncertainties in mechanistic understanding

The rate of microbial copper sulphide production (if any) at the final swelling pressure remains to be determined. Rate limiting factors such as diffusion of nutrients and sulphide, radiation, water content and heat stress must be clarified and defined.

Migration of microorganisms through compacted bentonite is not well studied. The restrictions due to a low pore size may need to be experimentally defined.

Formation of biofilms on the canister surface has been suggested to occur. This may be the case during the initial swelling phase. However, those microorganims will obey the same restrictions as any microbe in other parts of the buffer. The stress factors will be more severe at the canister surface than anywhere else in the buffer.

The mechanisms for survival of microbes in bentonite and buffer materials are not fully understood. Evidence for the presence of viable microbes in commercial MX-80 bentonite suggests that SRB and also other species can withstand the very dry conditions (10%) in commercial bentonite. The present hypothesis is that microbes are introduced to the clay during mining and processing. The clay causes dehydration, which will gently remove water from the cell. The cells will be inactive, but viable. This process is similar to freeze drying of cells, which also results in inactive but viable cells, e.g. freeze dried bakers yeast. Adding water revives the microbes to an active life.

The observed disappearance of microbial activity and viability in highly compacted bentonite under repository conditions is hypothesised to be a combined effect from desiccation and mechanical pressure and other stress factors. The sum of stress factors, radiation, heat, low water availability and a high mechanical pressure results in death of the microbes. However, the exact mechanisms for the observed disappearance of viability of microorganisms remain to be clarified.

Model simplification uncertainties

Not relevant since a model for microbial processes in the buffer is lacking.

Input data and data uncertainties

Not relevant since a model for microbial processes in the buffer is lacking.

2.5.14 Speciation of radionuclides

Overview/general description

Speciation of radionuclides is of importance for sorption and diffusion in the buffer. It is influenced by what speciation the nuclide had at the boundary to the buffer, i.e. inside the canister, but also by the chemical conditions in the buffer.

Table 2-22 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Boundary conditions

The boundary condition for the process in the source term from the canister/fuel, ie the speciation inside the canister.

Model studies/experimental studies

If the water chemistry in the buffer is known, the speciation of radionuclides can be calculated with a thermodynamic equilibrium model, like PHEEQC or EQ3/6 together with a relevant thermodynamic database.

Table 2-22. Process/variable table for the process Speciation of radionuclides.

Variable	**Does this variable influence the process?**		**Does the process influence this variable?**	
	Influence present?	**Handling of influence?**	**Influence present?**	**Handling of influence?**
Buffer geometry	No		No	
Pore geometry	No		No	
Radiation intensity	(The effect from radiolysis in the buffer will be small)		No	
Temperature	Yes	The uncertainty with respect to temperature is considered	No	
Water content	Indirect influence on speciation, because porewater composition changes with water content		No	
Gas content	No		No	
Hydrovariables (pressure and flows)	No		No	
Stress state	No		No	
Bentonite composition	Via pore water		No	
Montmorillonite composition	Via pore water		(Sorbed radionuclides will change the smectite composition, but the effect is limited)	
Pore water composition	Yes	Used in calculation	Yes	Results from calculations
Structural and stray materials	Yes	Not considered within SR-Can	No	

Time perspective

All, but only if there is a canister failure

Natural analogues/observations in nature

Not applicable.

Handling in the safety assessment SR-Can

The solubility and speciation of radionuclides is calculated and used as a source term for the modelling of release from a defective canister (See /process report fuel processes/). This is done for a wide span of water compositions.

In the buffer, the speciation is used to determine the transport properties of the radionuclides. However, the parameters for the transport properties used in SR-Can are selected based on experiments done under relevant conditions or from thermodynamic sorption models. See Section 2.5.5 and 2.5.3. The consistency of these speciations with the speciation calculated in the source term will be checked.

Uncertainties

Uncertainties in mechanistic understanding

See processes Section 2.5.5 and 2.5.3.

Model simplification uncertainties for the above handling in SR-Can

See processes Section 2.5.5 and 2.5.3.

Input data and data uncertainties for the above handling in SR-Can

See processes Section 2.5.5 and 2.5.3. There may also be uncertainties in thermodynamic data. This is discussed in /SKB 2006f/.

2.6 Radionuclide transport processes

2.6.1 Transport of radionuclides in water phase

Overview/general description

A number of processes will or could influence the transport of radionuclides in the water phase:

- advection, if the hydraulic conductivity of the buffer is high
- diffusion, will generally be the main transport mechanism through the buffer
- sorption, will have a strong effect on the transport on most radionuclides
- speciation, will determine how the radioelements are sorbed and transported
- colloid transport, could enhance the transport of radionuclides
- radioactive decay, will determine how much of the inventory of the radionuclides that eventually will leave the buffer.

All these have been discussed among the processes occurring in the buffer above, or, in the case of decay, under fuel processes.

Table 2-23 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Table 2-23. Process/variable table for the process Transport of radionuclides in water phase.

Variable	Does this variable influence the process?		Does the process influence this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Buffer geometry	Yes	Geometry is included in RN-transport calculations	No	
Pore geometry	Yes	Determines diffusivity, see 2.5.3	No	
Radiation intensity	No		No	
Temperature	Yes	Neglected RN-transport occurs after thermal pulse	No	
Water content	(No)	Radionuclide transport is assumed to take place when the buffer is saturated	No	
Gas content	(No)	Radionuclide transport is assumed to take place when the buffer is saturated	No	
Hydrovariables (pressure and flows)	Yes	Near field flow is considered in calculations	No	
Stress state	No		No	
Bentonite composition	Yes	See 2.5.5	No	
Montmorillonite composition	Yes	See 2.5.5	(By cation exchange)	Neglected since effect from radionuclides is small
Pore water composition	Yes	See 2.5.6	Yes	Output from RN-calculations
Structural and stray materials	No	Indirectly through porewater	No	

Boundary conditions

The inner boundary for this process is the gas pressure within a defective canister. The outer boundary is the fractures in the wall of the deposition hole.

Model studies/experimental studies

Not done for relevant conditions.

Natural analogues/observations in nature

Not relevant.

Time perspective

The process is active at all timescales after canister failure.

Handling in the safety assessment SR-Can

Radionuclide transport in the buffer is handled in the integrated modelling of radionuclide transport for the repository.

Model: The near field code COMPULINK/COMP23 /Romero et al. 1999/ will be used for the calculations. The code calculates the non-stationary nuclide transport in the near field of a repository. The system is divided into compartments, where the only restriction is that a compartment is formed of the same material. The model, which is basically a coarsely discretised Integrated Finite Difference Model, embeds analytical solutions at locations which otherwise would require a very fine discretisation, such as entrances and exits from small holes and fractures. In the repository, radionuclides leaking out through a small hole in the canister wall diffuse into the buffer and then may migrate through various pathways into the flowing water in the rock fractures.

The buffer processes that need to be considered are treated in the following way:

- **Advection** is neglected if the buffer conductivity is $< 10^{-12}$ m/s, see 2.3.2.
- **Diffusion** is treated with element specific diffusivities and porosities, see 2.5.3.
- **Sorption** is treated with linear sorption coefficients (Kd) for all elements, see 2.5.5.
- **Colloid transport** is neglected in the buffer, provided the buffer completely envelops the canister and has a dry density of at least 1,000 kg/m^3, i.e. a clay density of at least 1,650 kg/m^3, see 2.5.4.
- **Speciation of radionuclides** is directly included in the calculation of the source term from the inner boundary condition. The speciation is also included in the determination of the sorption coefficient.
- **Radioactive decay** and chain-decay are considered in the calculations.

Boundary condition: Radionuclide transport in the buffer is strongly dependent on the conditions at the inner and outer boundaries. The geometry of defects and fractures will determine the rate of transport.

Handling of variables influencing this process: The buffer geometry is included as compartments in the model. The buffer variables montmorillonite composition, bentonite composition and porewater composition will together determine the transport parameters. These include: porosity, diffusivity and sorption coefficients.

Handling of variables influenced by the process: The concentrations and mass flows of radionclides are calculated.

An earthquake of large magnitude may potentially change the boundary conditions for the process, while the radionuclide transport within the buffer will remain the same.

A simplified, analytic model /Hedin 2002/ will be used for scoping calculations of radionuclide transport in the near-field. This model is built on the same conceptual understanding of radionuclide transport in the buffer as COMP23.

Uncertainties

Uncertainties in mechanistic understanding

This process is an integration of several other processes all of which have uncertainties (see above).

Model simplification uncertainties for the above handling in SR-Can

The COMPULINK/COMP23 code uses rather a coarse discretisation of the buffer and analytical solutions for the boundary conditions at the canister and the rock.

Input data and data uncertainties for the above handling in SR-Can

The data uncertainties for the transport parameters in the buffer are presented in process 2.5.5 and 2.5.3. All input data to the radionuclide transport calculations will be handled in the SR-Can data report.

2.6.2 Transport of radionuclides in gas phase

A pulse of hydrogen gas can be released from a defective canister see Section 2.3.3. Some radionuclides could potentially enter the gas phase and thereby be transported to the surface much more rapidly than would be the case for the aqueous pathway. In principle, only C-14 and Rn-222 can enter the gas phase.

Overview/general description

Table 2-24 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Boundary conditions

The inner boundary for this process is the gas pressure within a defective canister. The outer boundary is the fractures in the wall of the deposition hole.

Table 2-24. Process/variable table for the process Transport of radionuclides in gas phase.

Variable	Does this variable influence the process?		Does the process influence this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Buffer geometry	(Yes)	See 2.3.3	No	
Pore geometry	No		No	
Radiation intensity	No		No	
Temperature	(No)	The thermal phase will be over before high enough gas pressures can be reached	No	
Water content	No		No	
Gas content	(No)	The process is assumed to occur only when the buffer is saturated	Yes	Output from transport estimate
Hydrovariables (pressure and flows)	The gas pressure will be dependent on the hydrostatic pressure	The pressure build up determines the time for gaseous releases	No	
Stress state	The opening pressure is dependent on the swelling pressure	The pressure build up determines the time for gaseous releases	No	
Bentonite composition	(Indirect via stress state)		No	
Montmorillonite composition	(Indirect via stress state)		No	
Pore water composition	(Indirect via stress state)		No	
Structural and stray materials	No		No	

Model studies/experimental studies

Not done for relevant conditions.

Natural analogues/observations in nature

Not relevant.

Time perspective

The process will only occur if there is a defect in a canister and if a sufficient amount of water is supplied to the iron insert to generate, over time, a gas pressure that is higher than the opening pressure of the bentonite.

Handling in the safety assessment SR-Can

Radionuclide transport in a gas phase will be treated as a separate case in SR-Can. The handling is based on the experiment by /Harrington and Horseman 2003/ presented in Section 2.3.3. It is assumed that if gas production exceeds the ability of the surrounding groundwater to take it into solution and transport it away from the container that pressure will build up within and adjacent to the container. The bentonite is assumed to ultimately open and release gas when the internal pressure exceeds 20 MPa. A rapid outflow will occur until the pressure falls to 10 MPa. This means that half of the gas inside the canister will be released instantaneously together with the radionuclides contained in that amount of gas. The only important radionuclide that can be transported in a gas phase is C-14. Since its half-life is 5,568 years, neither the buffer nor the geosphere is expected to significantly delay the transport to the biosphere.

The pathway is expected to stay open as long a there is a gas production in the canister (see 2.3.3). After the breakthrough pulse the gas is expected to be released at the same rate as it is produced by corrosion.

Uncertainties

Uncertainties in mechanistic understanding

The mechanisms for gas release through bentonite are still not fully understood, see Section 2.3.3.

Model simplification uncertainties for the above handling in SR-Can

The handling of the gas transport pathway in SR-Can is based only on a few experiments. The values for opening and steady state pressures have been selected on from those experiments.

Input data and data uncertainties for the above handling in SR-Can

As mentioned above, the values for gas opening and state pressures are based on experimental evidence. However, under any conditions, the gas pressure differential should be in the range of 5–15 MPa. Another uncertainty is the fraction of C-14 that can enter a gas phase. In the safety assessment SR 95 /SKB 1995/, the value of 3.5% was selected based on /Codell 1993/. This value may be associated with a large uncertainty, since the chemical form of carbon remains uncertain. In SR-Can it is assumed that the entire inventory of C-14 can enter the gaseous phase. For Rn-222, it is probably fair to assume that all of the inventory will be in the gas phase.

3 Processes in the deposition tunnel backfill

3.1 Thermal processes

3.1.1 Heat transport

Overview/general description

Heat is transported from the canister surface to the buffer, through the buffer and finally from the buffer to the rock, both directly and via the tunnel backfill. The canister power, the canister spacing and the rock thermal properties determine the thermal evolution within the backfill, while the thermal processes in the deposition holes and the temperature distribution in the buffer are unimportant.

The heat conductivity of the repository host rock is in the range of 2.5–3.6 W/(mK) /SKB 2005ab/. The backfill conductivity is usually set at 1.5 W/(mK) /Börgesson and Hernelind, 2000/. This means that the conductivity of the surrounding rock is about twice that of the backfill. In addition, the volume fraction of the heated near-field that is occupied by the backfill is small. These facts together mean that the thermal conditions in the backfill are dominated and controlled by the temperature of the surrounding rock and that details in the backfill heat transport properties are unimportant to the overall thermal development in the near-field. The disturbance induced by the presence of the low conductivity tunnel backfill will be small.

For a typical case the temperature increase may be about 40°C in the tunnel floor region and about 35°C in the roof region. The floor-roof gradient may be 2°C/m at maximum. After 100 years, the gradient is less than 1°C/m (Figure 3-1). In central parts, thermal gradients along the tunnel axes are much smaller and disappear after a couple of years. Close to tunnel faces and to sealing plugs, these gradients will be larger. Similar to the conditions in the buffer, the majority of the heat transport within the backfill will take place by conduction with thermal conductivities that depend on void ratio and saturation. While the buffer thermal conductivity and variations in buffer conductivity are important to the buffer temperatures, corresponding conditions in the backfill do not have much influence on the backfill temperatures.

Table 3-1 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Backfill geometry: The geometry of the backfill is defined by the shape of the excavated tunnels and possibly by formation of small gaps below the roof. None of these conditions can be expected to change in a way that can affect the heat transport in the backfill. There will always be sufficient backfill/rock contact to ensure that the rock and the backfill are in thermal equilibrium.

Backfill pore geometry: The thermal conductivity varies with the void ratio. The thermal expansion will affect the void ratio very insignificantly.

Temperature: The influence of heat transport on the backfill temperature is obvious. Different models have been proposed for estimating the influence of the temperature on the thermal conductivity of bentonite /Knutsson 1983/. Similar models could be applied to the backfill. The effect is a small but uncertain increase, which can be conservatively ignored.

Table 3-1. Process/variable table for the process Heat transport.

Variable	Does this variable influence the process?		Does the process influence this variable?	
	Influence present?	**Handling of influence?**	**Influence present?**	**Handling of influence?**
Backfill geometry	No		No	
Backfill pore geometry	Yes	Neglected, since the thermal expansion will affect the void ratio very insignificantly.	Indirectly via temperature (and thermal strain)	
Temperature	No	ignored	Yes	Result from the model (in time and space)
Water content	Yes	Insignificant in comparison to effects of other processes	No	ignored
Gas content	Indirectly through water content		No	
Hydrovariables (pressure and flows)	No		Indirectly via temperature	
Stress state	No	Ignored	No	Indirectly via temperature (and thermal strain)
Backfill composition	Yes	Backfill thermal conductivity given as input data	No	
Backfill pore water composition	No		No	
Structural and stray materials	No	Ignored	No	

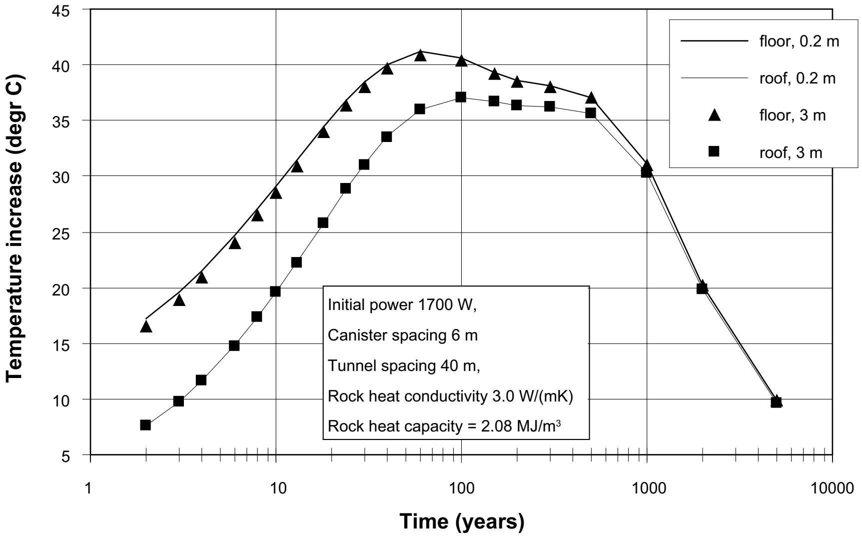

Figure 3-1. *Temperatures in tunnel floor and tunnel roof for two positions: 0.2 m and 3 m, respectively, from the axis of the nearest canister. Temperatures are calculated with analytical solution given by /Claesson and Probert 1996/ without regard to the properties of the backfill.*

Water content: The conductivity-saturation relations that apply for the buffer are in principle valid also for the backfill, i.e. there is dependence on the water content (cf Equation 3-1, /Knutsson 1983/). The parameter values of the equation will depend on the backfill composition.

$$\lambda = \lambda_0 + K_e (\lambda_1 - \lambda_0) \qquad (3\text{-}1)$$

where

λ_0 = thermal conductivity at $S_r = 0$ (dryness)

λ_1 = thermal conductivity at $S_r = 100$ percent (water saturation)

$K_e = 1 + \log S_r$

Both λ_0 and λ_1 depend on the void ratio.

A small fraction of the heat flow given by Equation 3-1 may be due to convection rather than to pure conduction.

The thermal gradients within the backfill are much smaller than in the buffer. The temperatures are low in comparison to those found in the buffer. Therefore any thermally driven redistribution of water from the floor region to the roof region during the time period of incomplete saturation is judged to be insignificant in comparison to effects of other processes that control the state of saturation in different parts of the backfill.

Gas content: The heat transport will not affect the gas content. The gas content in itself does not have any influence on the heat transport. If there is a gas phase, the effects of this will be just those of the incomplete saturation.

Hydro variables: Temperature variations will cause changes to the pore water pressure and initiate some convective flow.

Backfill geometry: The geometry of the backfill is given by the shape of the excavated tunnels and possibly by formation of small gaps below the roof. None of these conditions can be expected to change in a way that can affect the heat transport in the backfill. There will always be sufficient backfill/rock contact to ensure that the rock and the backfill are in thermal equilibrium.

Backfill pore geometry: The thermal conductivity varies with the void ratio. The thermal expansion will affect the void ratio very insignificantly.

Stress state: There may be some increase of the backfill thermal conductivity when stresses increase, but the effect is not sufficiently verified to be credited /Börgesson et al. 1994/. The increased temperature will induce some thermal stresses.

Backfill composition: The composition of the backfill will influence the thermal conductivity. Some minerals have higher conductivities than others.

Backfill porewater composition: No influences.

Impurity content: The presence of impurities may affect the thermal conductivity. To be of any importance, the impurity content must be high and the thermal properties of the impurities significantly different from those of the backfill.

Structural and stray materials: To be of any importance to the heat transport, there must be very significant amounts of non-backfill materials.

Boundary conditions

The tunnel peripheries, the tunnel faces and sealing tunnel plugs are the boundaries of the backfill. These boundaries are all approximately in thermal equilibrium with the host rock which changes its temperature slowly as a result of the decreasing heat output from the fuel, buried a couple of meters below the tunnel floor, and the transport of heat from the nearfield to the geosphere boundaries. The temporal and spatial variation of the rock temperature is conceptually well understood.

Model studies/experimental studies

Model studies. There are no studies that explicitly address the thermal conditions in the backfill. Because of its small importance and its weak coupling to other processes, modelling results from this process are available only indirectly from studies that address thermal issues in general. Predictions of the temperature evolution in the near field have, for instance, been done analytically /Claesson and Probert 1996, Hökmark and Fälth 2003, Hedin 2004/ and numerically /Thunvik and Braester 1991, Hökmark 1996, Ageskog and Jansson 1999/.

Natural analogues/observations in nature

Not applicable.

Time perspective

The duration of the thermal pulse is a few thousand years. The general statements made for the thermal pulse hold also during following phases, i.e. heat transport in the backfill is completely controlled by the thermal development of the host rock. Effects of climate changes and variations in geothermal heat flow will be imposed on the backfill by the surrounding rock.

Handling in the safety assessment SR-Can

There is no specific handling of heat transport in the backfill during the thermal phase since the backfill temperature is not directly related to safety. Results from thermal analyses, obtained using either rock mass values or generic values of the backfill heat transport parameters, give sufficient information on the backfill temperature range during the thermal phase.

For permafrost and glacial conditions, the minimum temperature of the backfill is a concern, see further Section 3.1.2. For these conditions, the backfill temperature can be taken to be equal to that of the host rock. See further the SR-Can Geosphere process report /SKB 2006g/ for the treatment of rock temperatures for these conditions.

Uncertainties

Uncertainties in mechanistic understanding

There are no major uncertainties in mechanistic understanding. In the unsaturated state, the backfill is a system with solid, liquid and gas phases and obeys physical laws for such systems, but for practical purposes the heat transport is expediently described as pure conduction with a saturation-dependent or fixed conductivity.

Model simplification uncertainties for the above handling in SR-Can

Not relevant since the process is not modelled.

Input data and data uncertainties for the above handling in SR-Can

Not relevant since the process is not modelled.

3.1.2 Freezing

Overview/general description

The overview and general description of the corresponding buffer process, Section 2.2.2, are also valid for the backfill. However, backfill materials of bentonite/crushed rock mixture are more sensitive to freezing than the buffer since the bentonite density is lower, the healing properties less favourable and the hydraulic conductivity higher. The consequences for the backfill are thus expected to be more severe but of course not directly affect the canister.

The temperature at which the water in the backfill freezes is assumed to be 0 ˚C but is actually lowered compared to that of free water for three reasons:

- The water pressure at 500 meters depths causes a reduction in freezing point although it is small (about 0.5 degrees)
- The water structure in the bentonite is expected to reduce the freezing point but this effect is probably small in at least 30/70 backfill due to the low density of the clay phase
- The salinity of the groundwater may affect the freezing point

The actual freezing point and the consequences of freezing are not well known and will be studied. Based on that study, the temperature at which freezing occurs will be settled and the consequences both for a frozen backfill and after thawing will be judged. The temperature at repository depth will be evaluated over time in the handling of geosphere processes.

The potential effects in the backfill materials due to freezing and thawing are the same as for the buffer (Section 2.2.2).

Table 3-2 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Boundary conditions

If the backfill freezes, the water in the rock will also be frozen. This means that the availability of extra water during ice- lens formation within the backfill probably is very limited. Internal water redistribution is probably required.

The effect of freezing on the interaction with the buffer is not clear. There may be a competition for water.

Model studies/experimental studies

No studies on freezing of backfill materials done so far.

Natural analogues/observations in nature

No studies have been conducted. However, knowledge can probably be achieved by studying permafrost areas.

Time perspective

Freezing at repository depth is not expected for thousands of years. At this stage, the backfill is expected to be completely water saturated. This means that the effects may be severe since there is no space left for expansion of the water. Ice lens formation will take long time due to the low hydraulic conductivity of the backfill but if the freezing period extends over several centuries there will probably be consequences.

Table 3-2. Process/variable table for the process Freezing.

Variable	Does this variable influence the process?		Does the process influence this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Temperature	Yes	Freezing of backfill is not ruled out at this stage. However, the consequences of the process are not evaluated within SR-Can	(Freezing affects temperature)	
Water content	Via the freezing point and the transport capacity		Ice lens formation = accumulation of water	Freezing of backfill are not ruled out at this stage. However, the consequences of the process is not evaluated within SR-Can
Gas content	(A gas content would affect the process but the backfill will be completely saturated when freezing occurs)		No	
Hydrovariables (pressure and flows)	Water transport is involved in the process		Yes	Freezing of backfill are not ruled out at this stage. However, the consequences of the process is not evaluated within SR-Can
Backfill geometry	Via the distance to the boundary		(Insignificantly)	
Backfill pore geometry	Via the freezing point and the transport capacity		Yes	Freezing of backfill are not ruled out at this stage. However, the consequences of the process is not evaluated within SR-Can
Stress state	Affects the freezing point		Yes	Freezing of backfill are not ruled out at this stage. However, the consequences of the process is not evaluated within SR-Can
Backfill composition	Affects the freezing point		No	
Backfill pore water composition	Affects the freezing point		No	
Structural and stray materials	No		No	

Handling in the safety assessment SR-Can

A key issue is if freezing of the backfill can occur at repository level.

A separate study of the conditions needed for a freezing process in the buffer and backfill will as mentioned be done within SR-Can. See process 2.2.2

An analysis of the backfill of the tunnels and shafts extending from the repository to the surface is not included in SR-Can.

Handling of uncertainties in SR-Can

The long-term effect of freezing of backfill materials has not been investigated in an organised way, which means that there are many uncertainties.

3.2 Hydraulic processes

3.2.1 Water uptake and transport under unsaturated conditions

Overview/general description

Water transport in the backfill under unsaturated conditions is a complex process that is dependent on temperature, smectite content, degree of water saturation and water content in the different parts of the backfill. The most important driving force for water saturation under deep repository conditions is the external water pressure from the water in the rock fractures and the negative capillary pressure in the pores of the backfill that lead to water uptake from the surrounding rock. The hydraulic subprocesses are identical to those of the buffer (Section 2.3.1) and will not be reproduced in this discussion.

There are some differences in behaviour and parameter importance between the buffer and the backfill that it is valuable to point out:

Sub-process B2, transport of water in vapour form controlled and driven by a temperature gradient, is probably insignificant for a major part of the backfill due to the low temperature gradient. However, it can be of importance for the backfill just above the buffer in the deposition hole and lead to drying if the supply of water from the rock is small.

Sub-process E2, compression of air, can be an important factor in the water saturation process (Boyle's law) of the backfill. If the air is trapped, it must be compressed and go into solution in the water in order for water saturation to be achieved. In highly compacted bentonite, the suction potential appears to be sufficiently high for this to occur and full water saturation is achieved without any external water pressure. The 30/70 backfill, however, has such low suction that a pressurized air volume will remain if the air cannot seep out. A large part of the volume will disappear when full water pressure has developed due to compression of the air but remaining part of the entrapped air must be dissolved and diffuse out through the backfill and the rock.

Sub-process F1, transport of dissolved air in water. When trapped air is compressed during the water saturation phase, a portion of the volume is dissolved in the water. This solubility (Henry's law) is approximately 2 percent at air temperature but decreases rapidly at increasing temperature. In order for additional air to be dissolved, the dissolved air must be transported away, which takes place by diffusion. For backfill the rate of diffusion is mainly limited by the transport capacity (diffusion and flow) in the rock. If gases are dissolved in the groundwater in the rock the diffusion rate may be very low and the time to saturate the backfill very long.

Table 3-11 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

The table illustrates the complexity of this process since all variable influence the process and the process influence all variables but two.

Influence of salinity and temperature on wetting rate: These influences are practically the same as for water-saturated conditions and are described under that process.

Table 3-3. Process/variable table for the process Water uptake and transport under unsaturated conditions.

Variable	Does this variable influence the process? Influence present?	Handling of influence?	Does the process influence this variable? Influence present?	Handling of influence?
Temperature	Through water viscosity and temperature gradient		Wetting and drying affects thermal conductivity	Neglected since the effects are small in the backfill
Water content	Yes	Initial water content is given as input data in saturation calculation	Yes	State of saturation is calculated
Gas content	Yes	Initial gas content is given as input data in saturation calculation	Yes	State of saturation is calculated
Hydro-variables (pressure and flows)	Yes	Included variables in the saturation calculation	Yes	The pressure and suction is calculated
Backfill geometry	Yes	Given as input data in saturation calculation	Influencing through the swelling of blocks	See Section 3.3.1
Backfill pore geometry	Yes	Included in material data	Yes	State of saturation is calculated
Stress state	Yes	Included variables in the saturation calculation	Yes	The pressure and suction is calculated
Backfill composition	(Influenced through the retention curve)	Given as input data in saturation calculation	Unless via mineral conversion	Not relevant for saturation period
Backfill pore water composition	Yes	Given as input data in saturation calculation	Yes	See Section 3.4.4
Structural and stray materials	Insignificant	Excluded	No	

Influence of water and gas content: The hydraulic conductivity is strongly affected by the degree of saturation. A commonly used relation between hydraulic conductivity and the degree of water saturation is

$$K_p = S_r^{\,\delta} K$$

where

K_p = hydraulic conductivity of partly saturated soil (m/s)

K = hydraulic conductivity of completely saturated soil (m/s)

δ = parameter = 3-10 for backfill

S_r = degree of saturation (–)

The hydro-variables expressed as suction (negative pore water pressure) in an unsaturated backfill is strongly affected by the water content (retention curve) and the backfill composition. For 30/70 backfill the suction is low compared to for Friedland clay (and MX-80 at buffer density) since the clay matrix is determining the suction and the clay dry density in the ballast voids is low and the clay water ratio is high (clay dry density: dry mass of clay divided with net total volume available excluding the ballast grains; clay water ratio: mass of water divided with the dry weight of the clay). There is also an obvious difference between matric and total suction. Examples of measured suction in 30/70 backfill and in Friedland clay are shown in Figure 3-2 and Figure 3-3 (see /Johannesson et al. 2003/ and /Börgesson et al. 2006/).

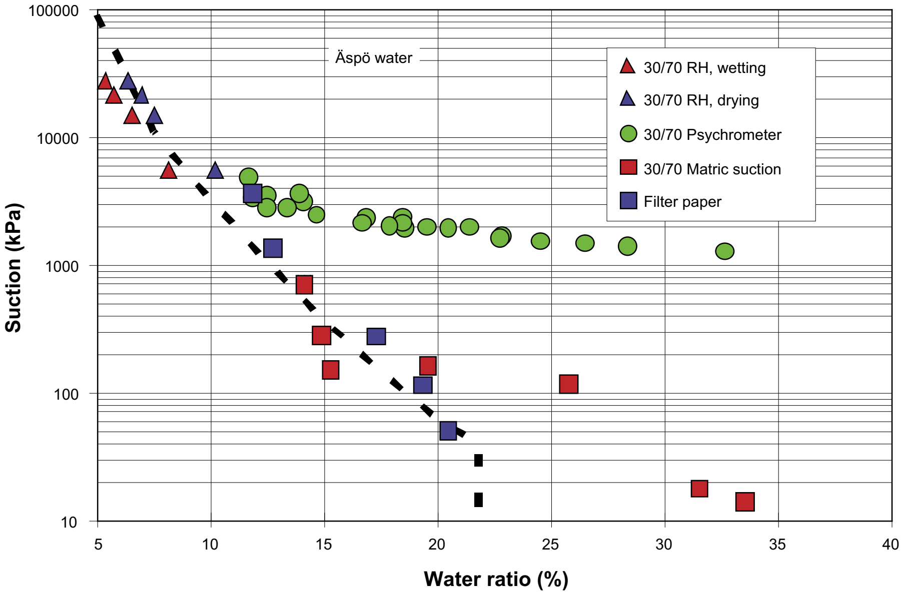

***Figure 3-2.** Measured relation between suction and water ratio for 30/70 backfill with 1.2% salt in the added water. The matric suction relation marked with the dashed line has been used in the calculations. The green dots represent total suction while the other results represent matric suction.*

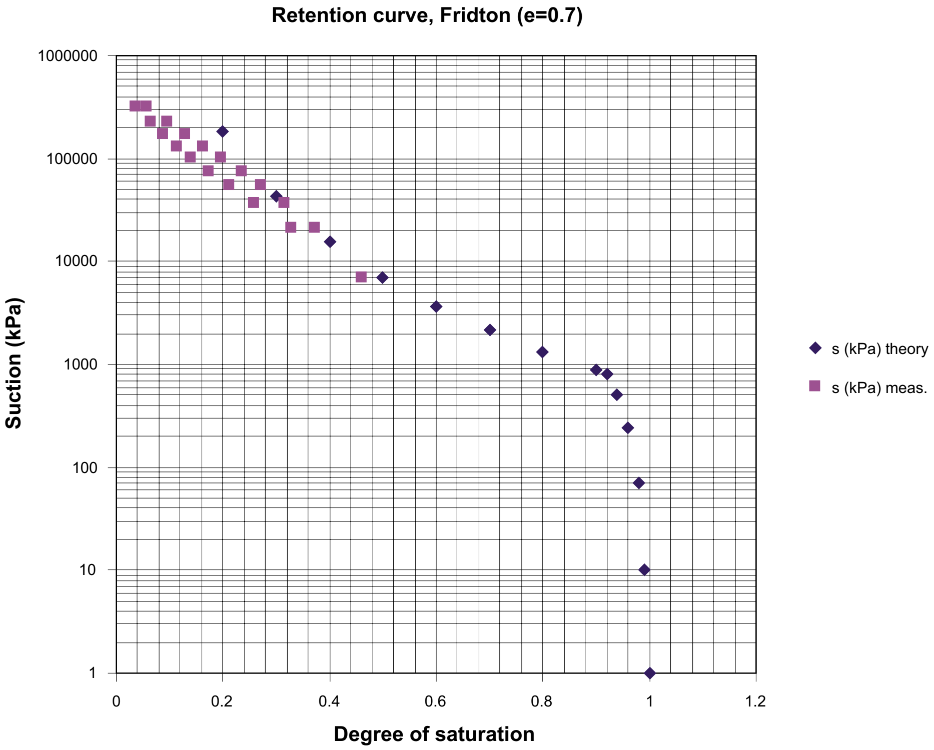

***Figure 3-3.** Measured and applied relation between suction and degree of saturation for Friedland clay at the void ratio 0.7, which corresponds to a dry density of 1,600 kg/m^3..*

The backfill geometry is of course affecting the wetting since the hydraulic gradient depends of the distance to the boundary. Usually the geometry is not affected by the wetting since the boundary of the backfill is the rock and the buffer, but if the backfill consists of different types of backfill (e.g. blocks and pellets) the geometry of the different types may change due to swelling or compression.

Boundary conditions

Interaction with the rock: A key issue for the saturation process is the interaction between rock and backfill. Water is conducted to the backfill in the water-bearing fractures and the rock matrix, which means that water saturation can be both uneven and take a long time for a sparsely fractured rock. If there is a highly permeable excavation-disturbed zone (EDZ) at the wall of the deposition tunnel, which distributes water from the fractures along the rock wall, the wetting will be faster and more even.

However, there is another process that may strongly increase the wetting rate of the backfill. When the water inflow from a rock fracture is stopped there will be an increase in the water pressure in the fracture. Since the backfill cannot withstand a high water pressure there will be piping and the water may flow in channels mainly along the rock surface but probably also into parts of the backfill. The water flow will partly be absorbed by the unsaturated pore system but as long as this absorption is slower than the water inflow the water will be further distributed along the rock surface due to the piping. This means that the wetting will be much faster than if it was caused by only water flowing through the matrix according to Darcy's law. This process is also treated in Section 3.2.4.

Interaction with the buffer: If the backfill is composed of a mixture of bentonite and crushed rock or similar material, the suction is much higher in the buffer material than in the backfill. This means that water will be transported from the backfill to the buffer and thus wet the buffer and dry the backfill. If the wetting of the backfill from the rock is faster than the wetting of the buffer, this water will also be redistributed to the buffer and thus help the wetting of the buffer.

Model studies/experimental studies

A preliminary material model containing unsaturated water flow has been derived (see /Böresson and Johannesson 1995/, /Börgesson and Hernelind 1999/) and is being further developed. The models were originally developed for buffer material and later adapted to backfill materials (see /Börgesson and Hernelind 1998/ and /Börgesson et al. 2006/). The calculations are performed using the finite element method with the program ABAQUS. See also the report about buffer processes. The model does not include the processes that handle air (except for B2 described above), which can be important for the saturation process in the backfill.

The model has been both calibrated and partially verified by laboratory experiments. The studies of the backfill material 30/70 have mainly been done within the project Backfill and Plug Test, while the models for buffer materials can be used for Friedland clay.

In recent years another finite element program has been tested and used for thermal and hydraulic processes, namely Code Bright /Cimne 2002/. This code is developed by UPC, Barcelona. Most processes are similar to the processes in ABAQUS but there are some important differences. The main difference is that it can handle the gas phase and thus also model processes B1, B4, B5, D2, E2 and F1. It can also handle phase transitions (C1 and C2).

Several large-scale field tests have been installed with i.e. the purpose to study the wetting process of the backfill material in a repository.

The big field test BMT (Buffer Mass Test) was performed in the years 1981 to 1985 in Stripa, Sweden (see e.g. /Gunnarsson et al. 2001/). In this test, highly-compacted bentonite and heaters were installed in six simulated deposition holes on a scale of 1:2. The tunnel above two of these holes was backfilled with sand-bentonite mixtures containing 10 and 20 percent bentonite. The tests were interrupted after a few years, whereupon buffer and backfill were excavated with detailed sampling and water ratio determination. The results showed that the wetting had gone to water saturation in the backfill 0.5 to 2 m into the backfill from the rock surface while there still were unsaturated parts in the centre of the tunnel.

In Äspö HRL there are two full scale projects for studying the processes in a backfill composed of 30% Na-bentonite and 30% crushed rock.

Backfill and Plug Test

The *Backfill and Plug Test* includes tests of backfill materials and emplacement methods and a test of a full-scale plug /Gunnarsson et al. 2001/. It is a test of the integrated function of the backfill material and the near field rock in a deposition tunnel excavated by blasting. It is also a test of the hydraulic and mechanical functions of a plug.

The main objectives of the Backfill and Plug Test are

- to develop and test different materials and compaction techniques for backfilling of tunnels excavated by blasting
- to test the function of the backfill and its interaction with the surrounding rock in full scale in a tunnel excavated by blasting
- to develop technique for building tunnel plugs and test the function

The entire test set-up with backfilling casting of the final part of the plug was finished in autumn 1999 and the water saturation, with water filling of permeable mats, started in late 1999. In the years up to 2001 the water saturation has continued and data from transducers were collected and reported. The plug was grouted and tested and in 2002 the water pressure in the permeable mats was increased to 500 kPa in order to shorten the time to reach full saturation. The backfill was water saturated in 2003 so the flow testing started in 2004. The models for unsaturated water flow in backfill material were evaluated and updated by the measurements done during the wetting phase. The flow testing done so far indicate that the hydraulic conductivity in the 30/70 is higher than required according to the criterion in Table 1-10.

Prototype Repository

The test location of the Prototype Repository is the innermost section of the TBM-tunnel at the –450 m level. The layout involves altogether six deposition holes, four in an inner section and two in an outer. The tunnels were backfilled with a mixture of bentonite and crushed rock (30/70). A massive concrete plug designed to withstand full water and swelling pressures separates the test area from the open tunnel system and a second plug separates the two sections.

Temperature, relative humidity, total pressure and pore water pressure are measured in a large number of points in the backfill (see e.g. /Börgesson et al. 2002/ and /Johannesson et al. 2004/). The measured results as well as the measurements after excavation will be used for evaluating the THM-models used for backfill materials.

Model studies

Besides the modelling of the Backfill and Plug Test and the Prototype Repository model studies of the saturation time of the backfill in a deep repository have been done for SR-Can /Börgesson et al. 2006/. The studies concerned the two backfill types 30/70 and Friedland clay. A large number of calculations of the wetting of the tunnel backfill with primary variations of fracture frequency, fracture transmissivity and backfill type and secondary variations of the rock matrix hydraulic conductivity, the distance to the water supplying boundary and the existence of a highly permeable zone at the rock surface has been done. The results are summarized in Figure 3-4 and Figure 3-5.

The following conclusions of these calculations were drawn:

The time to complete saturation varies according to the calculations from 0.5 years for 30/70 backfill and 1 m between fractures to more than 150 years for Friedland clay and 24 m between the fractures.

The influence of backfill type on the wetting rate is strong due to the difference in hydraulic conductivity of the different backfill types, which controls the wetting rate when the rock is highly fractured or permeable. The difference in time to full saturation of Fridton backfill is about 10 times longer than for 30/70 backfill in such a rock.

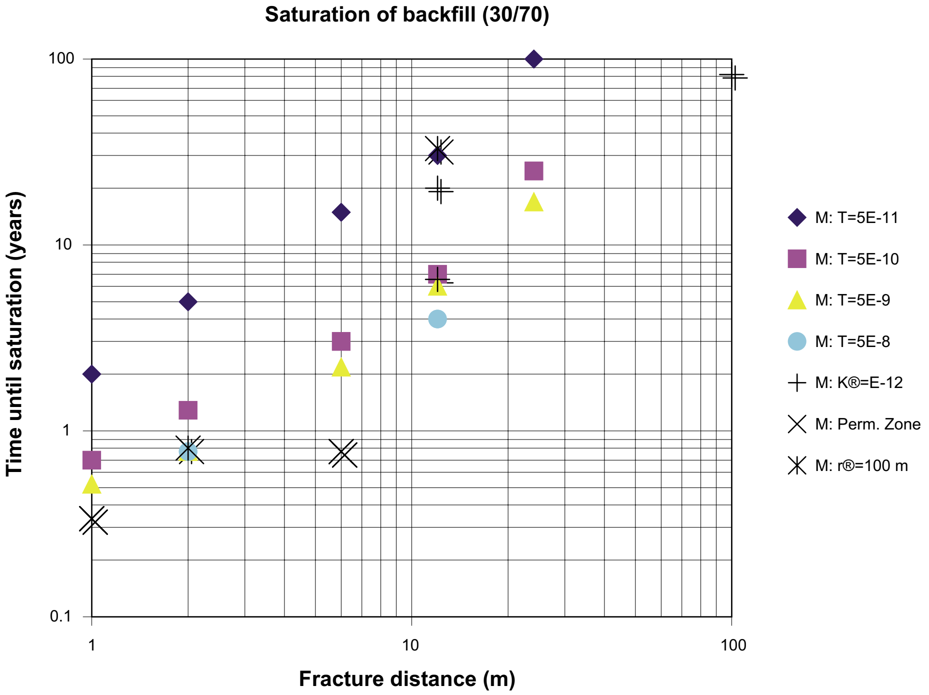

Figure 3-4. *Summary of results from calculations regarding 30/70 backfill with $K=0.5 \cdot 10^{-10}$ m/s in water saturated state. Influence of time until saturation as a function of the fracture distance at different fracture transmissivities T, rock matrix hydraulic conductivity ($Kr=10^{-13}$ m/s in all calculations except three). The influence of a highly permeable zone between the backfill and rock (or extensive piping) and a long distance to the hydraulic boundary (r_r=25 m for all other calculations) are alsoshown.*

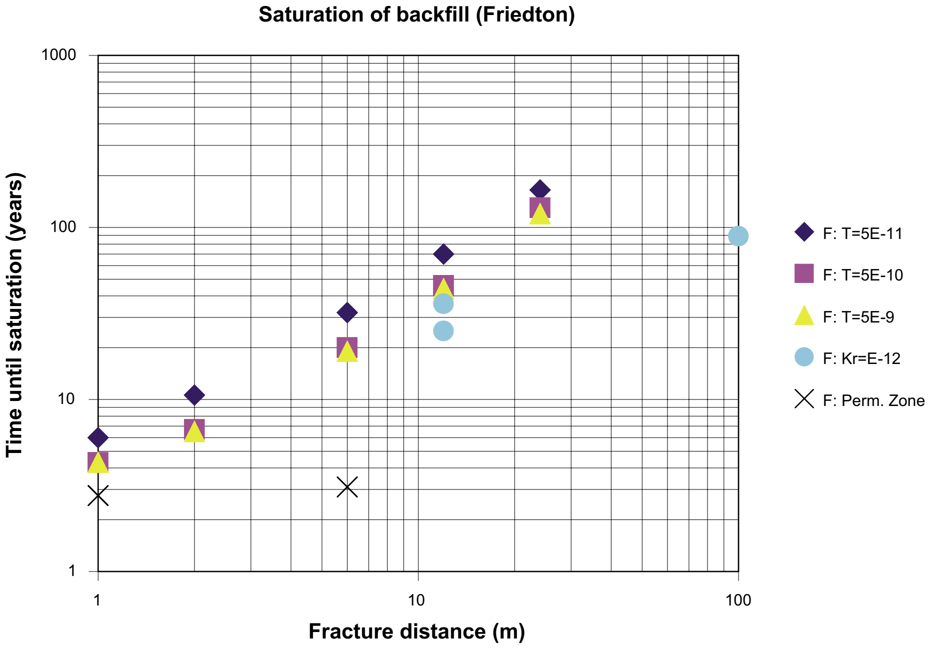

Figure 3-5. *Summary of results from calculations regarding Friedland clay backfill with $K=0.7 \cdot 10^{-11}$ m/s in water saturated state. Influence of time until saturation as a function of the fracture distance at different fracture transmissivities T, rock matrix hydraulic conductivity (Kr=10–13 m/s in all calculations except two). The influence of a highly permeable zone between the backfill and rock (or extensive piping) are also shown.*

The influence of fracture frequency is strong since very little water is transported in the rock matrix at the matrix hydraulic conductivity 10^{-13} m/s. The time to full saturation is almost proportional to the fracture distance.

The influence of transmissivity is insignificant except for the combination of the lowest transmissivity (T=10^{-11} m/s^2) and 30/70 backfill, since the transmissivity is high enough compared to the hydraulic conductivity of the backfill to yield a high water pressure in the fracture/backfill interface and the water inflow thus hindered by the backfill and not by the fracture.

The influence of a high matrix permeability (10^{-12} m/s instead of 10^{-13} m/s) is not very strong for the 30/70 and Fridton backfill since the average hydraulic conductivity including the fractures is not affected very much and the hydraulic conductivity of the backfills are still much higher than the hydraulic conductivity of the rock matrix.

Another conclusion is that the effect of piping can be very strong on the rate of wetting if the piping occurs between the backfill and the rock and produces a net of channels, since the channels will in such case function as a filter on the rock surface.

Natural analogues/observations in nature

Wetting of bentonite in nature has not been studied and can probably not contribute to the knowledge.

Time perspective

The above analyses show that the time to full water saturation of the backfill can vary a great deal, depending above all on the interaction with surrounding rock. If conditions are optimal for Swedish rock, saturation may be reached within 10 years. If there are no fractures all water has to go via the rock matrix, which may take 100 years in the granitic rock types occurring in Sweden.

Very long time until saturation of the backfill is not a problem for the backfill but the consequences in a very dry rock may be a delay of the water saturation of the buffer (see buffer processes).

Handling in the safety assessment SR-Can

As mentioned above, the initial THM evolution covering the saturation phase of the backfill has been modelled for a number of hydraulic boundary conditions in SR-Can since the supply of water at the outer buffer boundary is decisive for the wetting rate.

Model: The following sub-investigations have been made:

1. Investigation of the influence of the backfill properties and wetting conditions on the water saturation phase of the buffer with the old FEM-model used in earlier wetting calculations for SR-97. The old calculations have been updated regarding the influence of the backfill. 2D rotational symmetry.
2. Influence of the rock conditions on the wetting phase of the backfill in the deposition tunnels for three different backfill types. 2D rotational symmetry.
3. Influence of having entrapped air on the wetting phase of the backfill in the deposition tunnels. These calculations have bee done with Code Bright with a material model that includes the air phase. 2D rotational symmetry.

In addition to this, examples of complete interaction between buffer and backfill with a 3D model will be investigated. The results of the 2D calculations will be used for selecting a number of representative cases, which will be modelled in the 3D model and compared to the 2D models.

Timescales: The THM modelling will encompass the wetting period for the backfill. The detailed timescale will consequently be determined by the hydraulic conditions in the bedrock, which control the wetting. Typical timescales range from less than ten to more than a hundred years.

Boundary conditions: The THM modelling is performed for a number of different hydraulic conditions in the bedrock.

Handling of variables influencing this process: All the influences, except temperature, in the table above are included in the model.

Handling of variables influenced by the process: The degree of saturation (water content) in the backfill as function of time and space is calculated.

The special cases of failed canister and of earthquakes: Canister failures and earth quakes of a magnitude that could affect the wetting process are not expected during the time period in which the backfill saturates. The process is thus not handled for these cases. Should the assumptions regarding significant, early canister failures or earth quakes not be confirmed by the results of the safety assessment, the handling of the special cases will be reconsidered.

Uncertainties

The basic hydraulic properties of the backfill materials are rather well known. The main uncertainties of these properties concern the influence of salt in the groundwater and the influence of piping.

Uncertainties in mechanistic understanding

Just as mentioned under uncertainties of the buffer processes, there is a lack of understanding in how the high water pressure cause piping and distributes the water into the backfill from these channels. This process exists also in the buffer but it is much more important for the backfill since the buffer swelling pressure will rather soon seal the fracture (if the flow is not very strong) See also Section 3.2.4 (Piping/erosion).

Model simplification uncertainties for the above handling in SR-Can

The same model simplifications have been done for the backfill as for the buffer. Two of those are of higher concern for the backfill than for the buffer namely piping/erosion and inhomogeneities, since the homogenisation and self sealing processes are not as good in the backfill as in the buffer. These processes are dealt with in Section 3.2.2 (*Water transport under saturated conditions*) and Section 3.3.1 (*Swelling/mass redistribution*).

Input data and data uncertainties for the above handling in SR-Can

The greatest uncertainty/variability concerns the hydraulic conditions in the near-field rock and the hydraulic interaction between the rock and the backfill.

3.2.2 Water transport under saturated conditions

Overview/general description

Water transport under saturated conditions is mainly driven by a water pressure gradient. The process can be described by Darcy's law. Any deviations from Darcy's law, which can occur at low gradients, are favourable in that they lead to a reduced through flow rate. The hydraulic conductivity K depends on the composition of the buffer, the void ratio e, the ion concentration in the pore water i_c and the temperature T.

Water transport in saturated backfill is a complex interplay between several sub-processes on a microscopic scale. On a macroscopic level, the result is that the permeability of a saturated backfill is low, and this is also the essential result for the safety assessment.

Water flow in saturated backfill is a special case of unsaturated flow. The processes involved are the same as for unsaturated conditions.

The process is in general identical to the same process in the buffer and the behaviour is expressed by the hydraulic conductivity, *K*. The difference in hydraulic conductivity between the backfill and the buffer is mainly the magnitude. The influence of groundwater salinity is stronger for the backfill than for the buffer, since the clay density is lower (see 2.5.8).

The hydraulic conductivity of Friedland clay, one of the reference backfills, in non-saline water after complete saturation is approximately $2.0 \cdot 10^{-12}$ m/s at the dry density 1,700 kg/m^3 (2,070 kg/m^3 at water saturation). The influence of water salinity is rather strong. The corresponding hydraulic conductivity is about 5 times higher at a salinity of 3.5%. For the 30/70 backfill (mixture of 30% bentonite and 70% crushed rock), the other reference backfill, the hydraulic conductivity at the same density is $1.0 \cdot 10^{-11}$ m/s while the influence of salinity is very strong. The corresponding hydraulic conductivity is about 50 times higher at a salinity of 1.2%.

In order to prevent the deposition tunnels from being conductive pathways that influence the water movement in the in the repository, the backfill, shall over the entire length and cross-section of the tunnel, have a hydraulic conductivity that is in the same order of magnitude as that of the surrounding rock, or so low that diffusion is the dominating transport mechanism.

To meet this requirement, the demand of the average hydraulic conductivity of the backfill in the deposition tunnel has been set to $K < 10^{-10}$ m/s and the swelling pressure to > 100kPa to ensure a good contact with the rock wall /Gunnarsson et al. 2004./

Table 3-4 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Influence of density, temperature and water salinity:

The hydraulic conductivity is primarily dependent on the geometry and composition of the backfill, the density, the ion concentration in the pore water and the temperature.

For Friedland clay the influence of density and salt concentration in the pore water has been investigated /Pusch 2001, Johannesson and Börgesson 2002/ and the results are summarised in Figure 3-6.

For a 30/70 backfill the same type of relations /Johannesson et al. 1999, Johannesson 2004/ is shown in Figure 3-7. The results are from 3 different mixtures used at two different field tests at Äspö HRL:

- 30/70 mixed and saturated with distilled water
- 30/70 mixed and saturated with 0.7% salt water (Prototype Repository)
- 30/70 mixed and saturated with 1.2% salt water (Backfill and Plug Test)

The salt added to the water was NaCl and $CaCl_2$ in similar proportions.

The influence of a small percentage of salt in the water is much stronger for the 30/70 mixture than for both natural MX-80 and the natural Friedland clay. The reason is mainly the difference in clay type and clay density in the backfill. Clay density is defined as the average density of the clay material in the pores between the non-clay materials, i.e. the weight of the clay divided by the net volume (total volume minus the volume taken by the non-clay particles).

Table 3-4. Process/variable table for the process Water transport under saturated conditions.

Variable	Does this variable influence the process?		Does the process influence this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Temperature	Yes	The increase of hydraulic conductivity as function of temperature is about a factor 3 between 20°C and 90°C. This will be neglected in SR-Can because the thermal pulse will be over when any significant amount of radionuclides may have entered the backfill	No	
Water content	Influenced via density	Determines the hydraulic conductivity	No	
Gas content	No	Since the gases are solved the influence is negligible	(Advective transport of dissolved gases)	See 3.4.4
Hydrovariables (pressure and flows)	Yes	The hydraulic gradient determines whether advection can occur	Yes	Sensitivity analyses will be performed where the objective is to identify the parameter space where changes in conductivity result in large changes in performance.
Backfill geometry	Yes	Given as input data.	No	
Backfill pore geometry	Yes	Determines the hydraulic conductivity (see text) The pore geometry can be affected by a mineral transformation or a change in porewater composition. The effects are discussed in Sections 3.4.6 and 3.4.7	No	
Stress state	No		No	
Backfill composition	Yes	Determines the hydraulic conductivity (see text)	No	
Backfill pore water composition	Yes	Determines the hydraulic conductivity (see text)	Yes	Replacement of porewater is discussed in See 3.4.4
Structural and stray materials	Insignificant		No	

The clay density in the 30/70 backfill is low. At the dry density 1,700 kg/m^3 the clay dry density is about 900 kg/m^3 (1,600 kg/m^3 at saturation). The hydraulic conductivity of Na-bentonite is rather low at this density while there is a clear influence of the salt content in the pore water as well as a change in exchangeable cation from Na to Ca. In addition to this effect the influence of homogeneity of the clay phase in the backfill is strong. Investigations have shown that the clay is rather inhomogeneously distributed in the 30/70 backfill and the inhomogeneity increases with decreasing clay content /Börjesson et al. 2003/. This inhomogeneity means that large parts of the clay matrix have a much lower density than the average and are thus even more sensitive to salt.

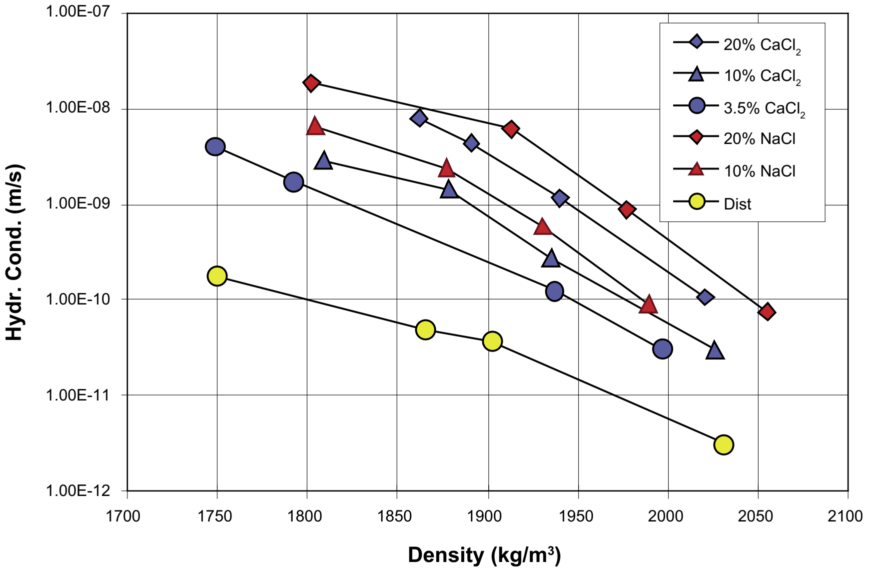

Figure 3-6. *Hydraulic conductivity of Friedland clay as function of the density at saturation at different pore water compositions of the saturating water. Initial water content 6–7%.*

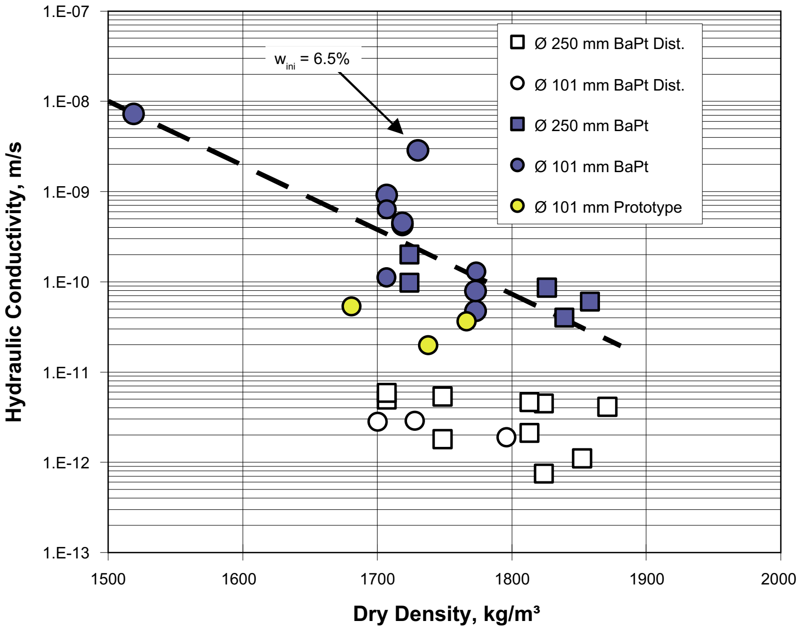

Figure 3-7. *Measured hydraulic conductivity as a function of dry density of 30/70 bentonite/crushed rock. The backfills are mixed and saturated with water with 0% salt (BaPt Dist) 0.7% salt (Prototype) and 1.2 salt% (BaPT).*

While the 30/70 backfill thus contains an inhomogeneous clay phase of Na-bentonite that is sensitive to salt, Friedland clay contains a much higher clay content with a clay that is more homogeneously distributed and clay minerals that are less sensitive to salt. All in all, these circumstances mean that the 30/70 backfill is more sensitive to salt in the groundwater than Friedland clay as shown in Figure 3-6 and Figure 3-7.

Transformations to other minerals resulting in reduced montmorillonite content generally lead to a higher hydraulic conductivity.

The temperature influences the conductivity by changing the viscosity of the water, whereby a temperature increase from 20°C to 90°C entails an approximate increase in conductivity by a factor of 3.

Boundary conditions

Only outer boundaries exist. There are three types of outer boundaries of the backfill in a deposition tunnel:

- The rock surface of the deposition tunnel and the upper metre of the deposition holes
- The interfaces between the backfill and the buffer in the deposition holes
- The inner surface of the concrete plug placed at the entrance of the deposition tunnels

The hydraulic conditions of these boundaries are very different. The hydraulic interaction with the rock after full saturation of the backfill is dominated by the hydraulic properties of the fractures in the rock. The hydraulic interaction with the buffer is governed by the hydraulic conductivity of the buffer. The interaction with the outer plugs is also complicated and depends on the tightness of the plug, the existence of a leakage through the rock/plug interface and the design of the plug. It may also change with time when the concrete degrades.

Model studies/experimental studies

Flow in water-saturated backfill has been studied on a laboratory scale in the form of permeability tests (se refernces above) and is presently studied on a full scale in the Backfill and Plug Test /Gunnarsson el al. 2001/. The latter full scale tests are presently running and evaluation is ongoing but preliminary results confirm the laboratory results and indicate that the hydraulic conductivity is high close to the roof and floor, mainly due to poor compaction at the roof and the interaction with the highly permeable disturbed zone in the floor caused by the rock excavation technique and the stress release due to the excavation.

In addition to these studies there is a project “Backfilling and closure of the deep repository” running. In this project the hydraulic conductivity of different backfill materials is investigated.

Natural analogues/observations in nature

No studies of water flow in natural backfill like formations have been done.

Time perspective

The hydraulic gradient that exists after closure of the repository when water saturation and pore pressure equilibrium in the backfill and surrounding rock have been reached is expected to be low. Since the backfill is designed to have a similar hydraulic conductivity to the rock the water flow in the backfill will be small. However, there is a time after closure of the deposition tunnel but before closure of the entire repository when there may be a rather high axial hydraulic gradient in the backfill. The axial water transport will during that time be largely depending on the tightness of the plug, the properties and geometry of the fractures in the rock around the plug and the possible existence of unhealed flow paths in the backfill caused by earlier piping and erosion. The latter flow paths are expected to be healed either during this period or just after pore pressure equilibrium has been reached.

Handling in the safety assessment SR-Can

Sensitivity analyses will be performed where the objective is to identify the parameter space where changes in conductivity result in large changes in performance. Thus, rather than assessing the influence of a few selected conductivity values, it is attempted to identify sensitive parameter transition regions.

Time periods: After saturation and throughout the assessment period.

Handling of variables influencing this process: The evolution of backfill density and composition together with the composition of the groundwater/porewater will be studied. The hydraulic conductivity and the swelling pressure will be evaluated for the changing conditions caused by the chemical evolution and alterations of density, section ##.

Handling of variables influenced by the process: The conductivity will be evaluated by application of the empirical relationships described above. The swelling pressure will be evaluated according to Section 3.3.1.

Boundary conditions: The hydraulic gradient for altered conditions during permafrost and glaciation will be estimated.

The special cases of failed canister and of earthquakes: Handled via possible mass redistributions, see Section 3.3.1. Consideration will also be given to pressure transients induced by earthquakes.

Uncertainties

Uncertainties in mechanistic understanding

Same as for the buffer (2.3.2).

Model simplification uncertainty

The model used is empirical connecting hydraulic conductivity to temperature, density and ionic strength of the pore water. The uncertainties in this description are primarily given by the uncertainties of the empirical relationships on which the model is based.

In addition there are two uncertainties, which are more important for the backfill than for the buffer. One is the above-mentioned effect of piping and erosion that may take place during installation and before final closure. These channels are expected to heal when the water flow is stopped and the backfill composition is designed for this. This ability of the backfill is checked in the present tests in the project “Backfilling and closure of the deep repository”.

Another uncertainty is the inhomogeneity of the backfill both in microstructure scale and in macro scale. The microstructure inhomogeneity (referring to particle localization) is primarily valid for the 30/70 mixture and is dependant on the mixing procedure. Careful instructions and control are required in order to avoid anisotropy in the backfill. The macro scale inhomogeneity is for in situ compaction caused by the problems related to compaction close to rock surfaces and for the backfill emplacement concept where blocks that are friction-fit together may experience incomplete swelling and homogenisation of the slots. All these uncertainties are investigated in the project: “Backfilling and closure of the deep repository”/Gunnarsson et al. 2004/.

Input data and data uncertainty

Same as for the buffer (2.3.2).

3.2.3 Gas transport/dissolution

Overview/general description

Transport of gas in the backfill can occur in two phases of the repository evolution:

1. Water saturation phase

The backfill will be emplaced with a water saturation of 40–80%, which means that there is a substantial amount of air that needs to be dissolved and transported away. Also the rock may contain dissolved gas. This was discussed in Section 3.2.1.

2. Gas transport from a defective canister after saturation

Hydrogen gas from the corrosion of the cast iron insert could potentially escape from the repository by transport through the tunnel backfill. /Wikramaratna et al. 1993/ has estimated the gas transport and gas storage capacity of the backfill. The backfill could act as a passageway for gas under certain conditions. However, it is not evident that gas from the canister will ever reach the tunnel. Gas release through the backfill is pessimistically neglected in SR-Can.

Table 3-5 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Boundary conditions

The rock may either be water unsaturated or completely water saturated. It may be unsaturated either by drying caused by low relative humidity in the tunnel or from gas dissolved in the groundwater (due to the pressure drop). If the rock is saturated it may include different amounts of dissolved gas.

Table 3-5. Process/variable table for the process Gas transport/dissolution.

Variable	Does this variable influence the process?		Does the process influences this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Temperature	Yes	Insignificant, since the temperature in the backfill will remain low	No	Insignificant
Water content	Via suction and degree of saturation		Yes	See 3.2.1
Gas content	Yes	See 3.2.1	Yes	
Hydro-variables (pressure and flows)	Yes	See 3.2.1	Yes	See 3.2.1
Backfill geometry	Yes	See 3.2.1	No	
Backfill pore geometry	Yes	See 3.2.1	Via swelling	
Stress state	Via suction		Via swelling	
Backfill composition	Yes	See 3.2.1	No	
Backfill pore water composition	Yes	See 3.2.1	No	
Structural and stray materials	No		No	

Model studies/experimental studies

The influence of trapped air on the saturation time has been studied in the SR-Can calculations (see /Börgesson et al. 2006/). Five 1D, axially symmetric models have been run with Code_Bright. Three different rock permeabilities were tried and in two of the models, a constant gas pressure has been assumed (no trapped air). The results yielded the following conclusions.

- If there are no escape routes for the air hosted in the initially unsaturated backfill other than through the host rock, the trapped air will have an impact on the saturation process. The trapped air forms a "bubble", which holds back the inflowing water and delays the saturation. This effect is more important the more permeable the rock is, since in a permeable rock, water enters faster than the gas can dissolve/diffuse away. When the water supply from the rock is high, the gas diffusion rate will control the water saturation process.
- Since the only way gas can escape is by being dissolved into the pore water and then diffuse away, the diffusion rate has a great importance for the saturation process. If the pore water in the undisturbed host rock contains considerable quantities of dissolved gas, the diffusion rate will be low with a correspondingly low saturation rate. If the rock is saturated with gas, the backfill will not be water saturated.

Natural analoges/observations in nature

Not applicable.

Time perspective

The delay of the water saturation of the backfill is relatively greater when the permeability of the rock is high rather than when it is low. However, since the saturation rate is only critical when the permeability is low the preliminary conclusion is that trapped air is not a very significant factor unless the rock is almost saturated with gas.

Handling in the safety assessment SR-Can

The influence of trapped air on the saturation time of the backfill is investigated in SR-Can. The process involving trapped air is only relevant during the saturation phase (see Section 3.2.1).

The escape of corrosion gas from the canister through the backfill is not considered in SR-Can.

Uncertainties

The parameter values for the modeling of the gas dissolution and transport are rather well defined. The largest uncertainty is the rock properties and the partly connected question of whether the air is trapped or not.

3.2.4 Piping/erosion

Overview/general description

Water inflow into the deposition tunnel will take place mainly through fractures and will contribute to the wetting of the backfill. However, if the inflow is localized to fractures that carry more water than the backfill can adsorb, there will be a buildup of water pressure in the fracture and therefore increase in the hydraulic gradient across the backfill. The backfill close to the rock surface initially either consists of pellets with low density (Friedland clay) or a bentonite-aggregate mixture with low swelling pressure (30/70). As a result the backfill will probably not be able to stop the water inflow due to the high water pressure that will be achieved in the fracture. The results may be piping, formation of a channel and a continuing water flow and erosion of soft bentonite gel or bentonite crushed rock mixture. The processes are described in Section 2.3.4 (buffer). The knowledge of this process and its consequences for the backfill are sufficient enough today. Research is ongoing (in the project Baclo /Gunnarsson et al. 2004/).

Piping is expected to take place in a lot of fractures in the tunnel for both concepts, since the swelling pressure of 30/70 backfill and bentonite pellets is lower than the expected water pressure, which means that it cannot resist the water pressure but will open a channel or a hydraulically initiated fracture.

The erosion is expected to be much stronger in the pellets than in the mixture due to the weight of the ballast particles.

For the 30/70 backfill the pipe is not expected to be closed until the water pressure gradient in the backfill has been reduced by the sealing ability of the plug at the end of the deposition tunnel. The limit is not known today. The plug and the sealing of leakages in the plug that may occur with time will reduce the flow rate and move the hydraulic gradient from the backfill to the plug, which will give the backfill time to selfheal. For Friedland clay the flow channels will be closed when the blocks have been sufficiently wetted to cause expansion and consolidation of the pellets, thereby yielding a sufficient resistance to erosion.

Influencing/Influenced variables

Table 3-6 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Boundary conditions

The piping and erosion that are treated here only take place in the pellets filled part between the Friedland clay blocks and the rock. For the in situ compacted bentonite/crushed rock mixture it is also likely that it mainly takes place in the interface between the backfill and the rock surface where the density is lower, but it may probably also spread into the central parts of the backfill.

Model studies/experimental studies

The processes are studied in conjunction with studies for KBS-3H, which is especially vulnerable for erosion of buffer material since a channel can pass a large number of canisters. Tests have been done at three different scales. The results show that the bentonite is very sensitive to piping and erosion and that it may take a considerable time until it heals if the inflow in one spot from a fracture is strong and the built-up of water pressure in the fracture is fast /Börgesson et al. 2005/.

At present the processes are studied in the project *Backfilling and closure of the deep repository* /Gunnarsson et al. 2004/.

Natural analogues/observations in nature

Not applicable for this process.

Time perspective

The piping and erosion only takes place before complete saturation and homogenisation in the Friedland concept. The high swelling pressure of the clay will ultimately always seal the piping channels, since the sum of the swelling pressure and the pore water pressure in the buffer will always be higher than the water pressure if the final average density of the clay is high enough. If the density is lower and in the 30/70 concept the flow must probably be stopped by the plug in the end of the deposition tunnel.

Table 3-6. Process/variable table for the process Piping/erosion.

Variable	Does this variable influence the process?		Does the process influence this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Temperature	No		No	
Water content	A change in water content changes the swelling pressure, which influences the piping risk. It also influences the hydraulic conductivity, which influences the swelling rate	Not taken into account – a conservative estimate is used	Piping may increase the saturation rate and thus affect the water ratio and degree of saturation since it may distribute the water in a more homogeneous manner via a net of pipes inside the backfill.	No effect of piping on the saturation rate of the backfill is considered. It could potentially speed up the saturation
Gas content	The degree of saturation and the porewater pressure in the backfill influences the risk of piping and the erosion rate	Not taken into account – a conservative estimate is used	Same as water content	
Hydro-variables (pressure and flows)	The degree of saturation and the porewater pressure in the backfill influences the risk of piping and the erosion rate	The effect of piping is evaluated with a simplified mass-balance approach	Same as water content	
Backfill geometry	The distance to the plug influences the water pressure gradient	The effect of piping is evaluated with a simplified mass-balance approach	No	
Backfill pore geometry	(Via density)		(In case of strong erosion)	
Stress state	Yes	The effect of piping is evaluated with a simplified mass-balance approach	Yes	The effect of piping is evaluated with a simplified mass-balance approach
Backfill composition	Yes	The effect of piping is evaluated with a simplified mass-balance approach	No	
Backfill pore water composition	The salinity of the water affects many variables that are important for disposion to piping and erosion, i.e. the swelling pressure, the swelling rate (through hydraulic conductivity) and the erodability	The effect of piping is evaluated with a simplified mass-balance approach	No	
Structural and stray materials	No		No	

Handling in the safety assessment SR-Can

Piping and erosion could lead to a loss or redistribution of the swelling clay component in the backfill. The implication of this is an increased hydraulic conductivity and a decreased swelling pressure.

In SR-Can the magnitude of this process will be estimated and the results will be used as an input for the water transport under saturated conditions (Section 3.2.2).

Time periods: The process is only relevant during saturation. The process is neglected for all other time periods.

Boundary conditions: The hydraulic boundary conditions at the backfill/tunnel wall interface are decisive for this process.

Handling of variables influencing this process: The water flow and the water pressure together with the water pressure increase rate are the key variables for this process. The erosion is also affected by the geometry of the initial slots in the system. The effect of the salinity of the groundwater is also included in the description.

Handling of variables influenced by the process: The consequence of an extensive piping together with erosion would be a localized loss of backfill density

The special cases of failed canister and of earthquakes: The process only occurs at very early stages when these special cases are not relevant.

Uncertainties

Piping, erosion and subsequent sealing is a complicated process with many components, much depending on the hydraulic behaviour of the rock. The uncertainty is thus very large regarding both the demands on the rock and the ability of the backfill to handle the processes. The tests performed for the backfill project are expected to yield better understanding. It is though probable that the end plug needs to be rather tight in order to stop the erosion especially for the 30/70 backfill.

3.3 Mechanical processes

3.3.1 Swelling/mass redistribution

The swelling process has been merged with other processes that cause mass redistribution within the backfill, namely thermal expansion, creep and a number of interactions with the buffer, near field rock and the plug.

Overview/general description

Water is absorbed by both unsaturated and saturated swelling backfill materials and causes swelling. If the backfill is unable to expand freely, a swelling pressure develops, which locally reaches its peak at full water saturation. The process is described in Section 2.4.1 about the buffer. The same basic process description is valid for the backfill.

Table 3-7 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Table 3-7. Process/variable table for the process Swelling/mass redistribution.

Variable	Does this variable influence the process? Influence present?	 Handling of influence?	Does the process influence this variable? Influence present?	 Handling of influence?
Temperature	Through thermal expansion	Excluded from assessment (see below)	(Insignificant)	
Water content	Yes	Included in THM modelling of unsaturated backfill	Yes	Included in THM modelling of unsaturated backfill
Gas content	Yes	Included in THM modelling of unsaturated backfill	Yes	Included in THM modelling of unsaturated backfill
Hydro-variables (pressure and flows)	Yes	Included in THM modelling of unsaturated buffer	Yes	Included in THM modelling of unsaturated buffer
Backfill geometry	Any phenomenon leading to alterations of the backfill bulk geometry influences swelling	The initial position of the backfill is the starting point of the evaluation	Yes	The backfill geometry after swelling is estimated
Backfill pore geometry	Indirectly through stress state		Indirectly through stress state	
Stress state	Yes	Included in THM modelling of unsaturated backfill	Yes	Included in THM modelling of unsaturated backfill
		Is included in calculation of the mechanical interaction with buffer		Is included in calculation of the mechanical interaction with buffer
Backfill composition	Yes	The initial composition of the backfill is the starting point of the evaluation	No	
Backfill pore water composition	Yes	The swelling pressure is given from the porewater composition	No	
Structural and stray materials	Yes	Not included in assessment	No	

The swelling pressure of the backfill is a function of all the variables included in the table. At present investigations of the swelling pressure of different backfill materials at different densities and pore water compositions are ongoing. Figure 3-8 shows a preliminary example of results on mixtures of 30% bentonite and 70% ballast material of crushed rock with a maximum grain size of 5 mm. Additional tests are ongoing. The swelling pressure of Friedland clay is considerably higher as shown in Figure 3-9 (see /Pusch 2001/ and /Johannesson and Börgesson 2002/). Despite the scatter there is an obvious influence of porewater salinity and composition.

Influence of **degree of saturation and temperature**: Same as for the buffer. See Section 2.4.1.

The influence of the **stress state** expressed as compression properties is important for the interaction with the buffer. Figure 3-10 shows the measured compression modulus (evaluated as the applied stress in an oedometer divided with the strain caused by the applied stress) as a function of the compaction energy expressed as % modified Proctor density for different backfill compositions /Johannesson et al. 2003/. Additional tests are ongoing.

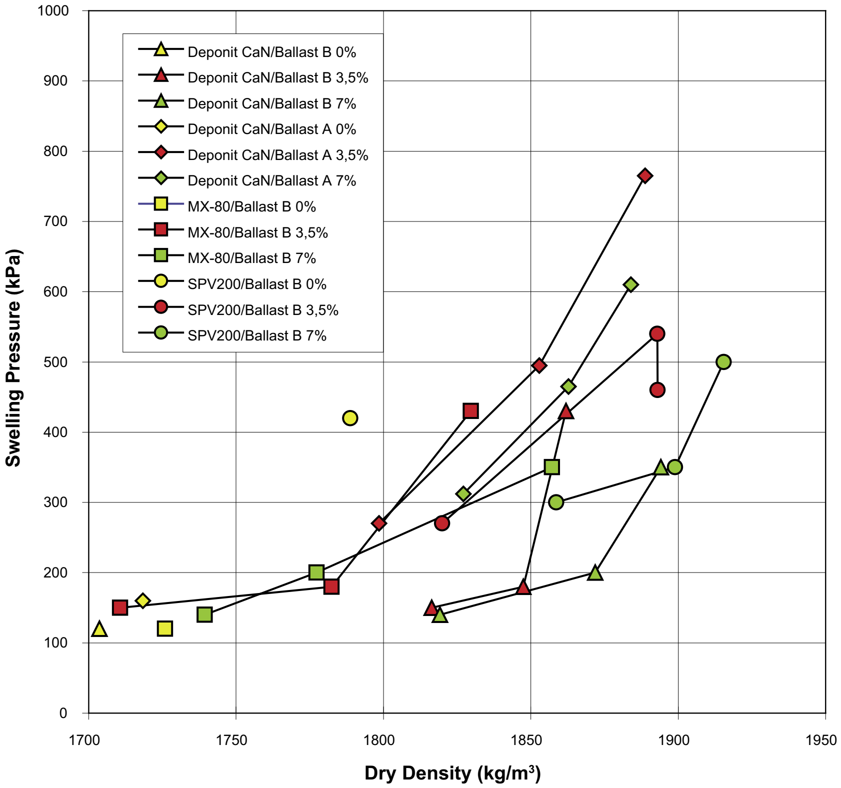

Figure 3-8. *Swelling pressure of a 30/70 mixture of Ca-bentonite and crushed rock as a function of dry density at different water salinities. Deponit CaN is a Ca-bentonite from Milos and SPV200 is a variant of MX80 (fine powder). The legend also shows the salinity of the water (50/50 CaCl/NaCl).*

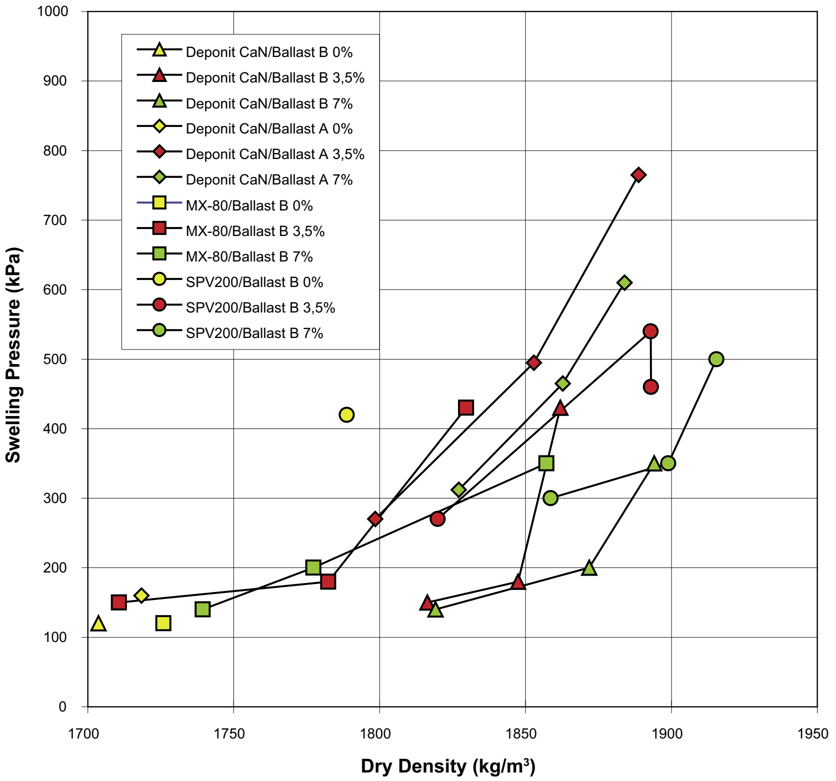

Figure 3-9. *Swelling pressure of Friedland clay as a function of dry density at different pore water salinity and porewater composition The legend show the salinity of the water added and the type of salt. Dist stands for distilled water.*

Figure 3-11 shows results of compression tests on Friedland clay but plotted as void ratio vs applied effective stress /Johannesson and Börgesson 2002/.

The results in Figure 3-10 and Figure 3-11 can be used for investigating the interaction between the backfill and the buffer and calculate the upwards displacement of the buffer/backfill interface.

Creep is not a very important factor for the backfill since it is smaller than for the buffer and does not affect the tunnel filling function of the backfill.

Boundary conditions

The backfill has three main boundaries, namely the buffer, the rock and the plug at the end of the deposition tunnel.

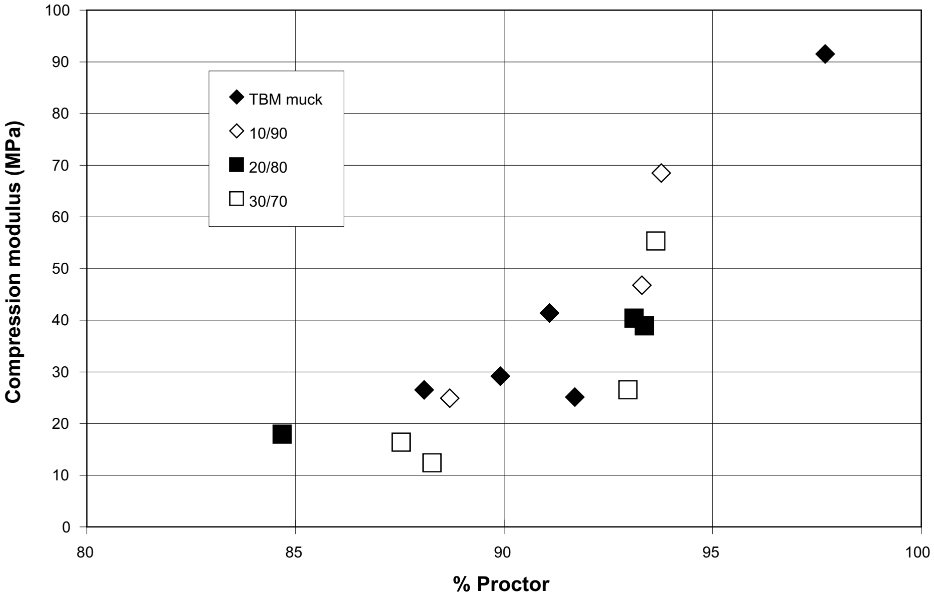

Figure 3-10. *Compression modulus as function of the compaction energy (% modified Proctor) for different mixtures of bentonite and crushed rock.*

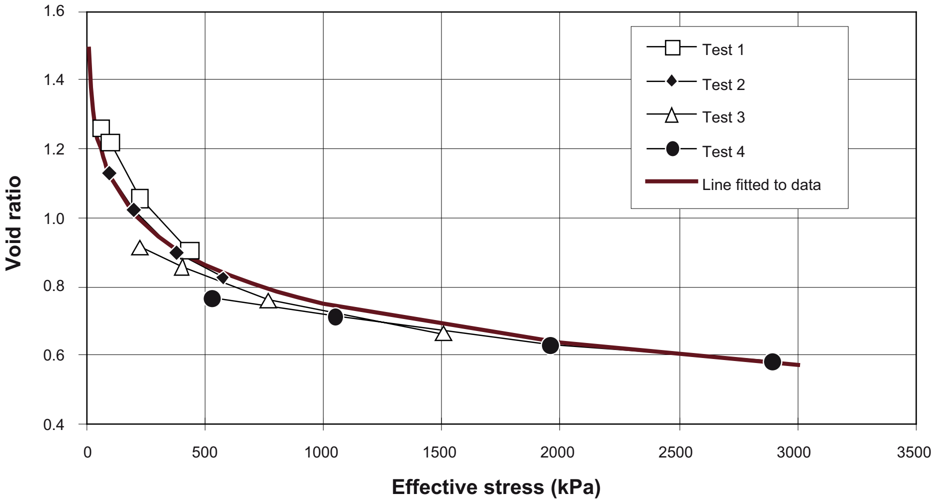

Figure 3-11. *Void ratio plotted as function of the vertical stress for 4 tests performed on Friedland clay.*

Interaction buffer/backfill

At the interface between the buffer and the backfill, the buffer exerts a swelling pressure against the backfill and vice versa. Since the difference in swelling pressure may be great, a net pressure arises against the backfill whereby the buffer swells and the backfill is compressed. In this process, the swelling pressure from the buffer decreases as the density decreases. At the same time, the counter-pressure from the backfill increases as it is compressed and its density increases. The swelling of the buffer and compression of the backfill are counteracted to some extent by friction against the rock. When the force of the swelling pressure in the buffer is equal to the sum of the force of the counter-pressure in the backfill and the friction against the rock, the process ceases since equilibrium has been established. The swelling of the buffer and corresponding compression of the backfill has been evaluated in the buffer chapter.

Interaction Backfill/Near field rock

The following mechanical interactions between backfill and near-field rock have been identified:

1. **Swelling pressure from the backfill** is transferred to the rock. The pressure is though rather low and is not expected to lead to significant rock movements. A positive effect is that the backfill supports the rock and helps keeping the rock surface unaffected.
2. **Swelling pressure from the buffer** is transferred through the backfill to the roof of the tunnel. The pressure is reduced by friction and load spreading and is not expected to harm the rock but rather support it in addition to the support according to item 1.
3. **Forces of friction** arise against the upper meter of the rock walls in the deposition hole due to swelling of the buffer against the backfill.
4. **Thermal expansion of the backfill** could be serious for the rock if the backfill is water-saturated when the temperature increase occurs. However, the slow temperature increase in combination with the drainage through the rock implies that this is not a problem.
5. **Convergence of the deposition tunnel** occurs when the rock creeps due to the high rock stresses after rock excavation. However, such convergence cannot affect the backfill negatively since it will only compress the backfill and increase its density. The concern arising from this process is the effect the creep has on the properties of the rock itself.

Intrusion of bentonite into fractures in the rock is very limited due to the small aperture of the fractures and the shear resistance caused by the friction between the backfill and the fracture surface. See the chapter about buffer.

Interaction Backfill/Plug

All deposition tunnels are likely to be ended with a water-tight plug. The mechanical influence from the swelling pressure is rather small compared to the influence from the water pressure that will prevail before closure of the repository. After closure, the water pressure will be equal on both sides.

Model studies/experimental studies

The swelling pressure and the compression properties of the two candidates for backfillare at present being investigated in the project "*Backfilling and closure of the deep repository*". The results are aimed at yielding enough information for estimating the required density of the backfill in the tunnels.

The only model studies done concerning mechanical processes in the backfill are the interaction buffer/backfill (see 2.4.1).

Three large-scale tests with backfill material have been installed (*BMT* in Stripa and *Backfill and Plug Test* and the *Prototype Repository* in Äspö HRL). In these tests the total stress from the swelling pressure of the backfill has been or is being measured. Also the displacement of the interface between the buffer and the backfill was measured in BMT and can be measured after excavation of the Prototype Repository.

Time perspective

Full saturation of the backfill and buffer is expected to be achieved within 100 years whereby the hydraulic conductivity of the rock is the limiting factor. This means that the stress equilibrium with full swelling pressure is expected to be achieved within that time. The creep of the backfill is small and can be neglected.

Natural analogues/observations in nature

No natural analogues concerning mechanical behaviour have so far been studied. The existence of relevant natural examples is probably very limited and would be difficult to evaluate.

Handling in the safety assessment SR-Can

One purpose of the backfill is to keep the buffer down in the deposition hole. The handling of the mechanical interaction between the buffer and the backfill in SR-Can is presented in Section 2.4.1.

It is important to ensure that there is a tight connection between the backfill and the tunnel wall. This is achived by the swelling pressure of the backfill material.

The evolution of backfill density and composition together with the composition of the groundwater/porewater will be studied. The hydraulic conductivity and the swelling pressure will be evaluated for the changing conditions caused by the chemical evolution, Section 3.4.4 and alterations of density, Sections 3.2.4 and 3.4.7. The conductivity will be evaluated by application of the empirical relationships described above. The swelling pressure will be evaluated according to Section 2.4.1.

Uncertainties

Uncertainties in mechanistic understanding

After complete water-saturation, the swelling process is deemed to be sufficiently well-known and the final density distribution in the backfill can be calculated with sufficient accuracy. In the long-term perspective the swelling properties can change due to transformations and cementation. These are chemical processes and treated in Section 3.4.7.

Model simplification uncertainties for the above handling in SR-Can

See above.

Input data and data uncertainties for the above handling in SR-Can

The largest uncertainty is probably the inhomegeneity of the in situ compacted backfill. The backfill will be considerably looser at e.g. the roof and close to the walls. There will be some homogenisation from the swelling but the low swelling pressure and the high friction in the backfill probably means that large density differences will remain.

3.3.2 Liquefaction

Overview/general description

Liquefaction is a process implying that a stiff material (soil) turns into liquid due to a distrubance of short duration. The process and consequences are described in the buffer chapter, Section 2.4.2. Just as for the buffer it is highly unlikely that it occurs in the backfill. If for any reason it should occur, the consequences for the backfill would be negligible, unlike for the buffer where the canister may tilt or sink to the bottom of the emplacement hole. The only conceivable effect is that a loose rock block in the roof may sink but the effect is local and since the total volume is constant the liquid backfill will fill the hole in the roof after the block moves.

Since the process is unlikely to occur and the consequences are negligible, the process will not be further dealt with.

3.4 Chemical Processes

3.4.1 Advective transport of species

Overview/general description

Solutes (dissolved substances) and colloids can be transported with the water in the backfill by pressure-induced flow: advection. Hereby, solutes move from areas of higher water pressure to areas of lower pressure. The process leads to redistribution of solutes in the water and thus affects the water composition. The main reason for a pressure gradient over the backfill is the hydraulic conditions (the topography) at the site. The advective transport of material is a direct function of water flow in the backfill, which is comprehensively described in Section 3.2.2.

Under certain conditions it is possible that the transport of solutes in the backfill will be dominated by diffusion (see Section 3.4.2).

Table 3-8 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Boundary conditions

The external boundary condition for this process is the gradient caused by the change in hydrostatic pressure across the backfill.

Model studies/experimental studies

Flow in water-saturated backfill has been studied on a laboratory scale in the form of permeability tests /Pusch 2001, Johannesson and Börgesson 2002, Johannesson et al. 1999, Johannesson 2004/ and is presently studied on a full scale in the Backfill and Plug Test /Gunnarsson et al. 2001/ The latter full scale tests are presently running and evaluation is ongoing but preliminary results confirm the laboratory results and indicate that the hydraulic conductivity is high close to the roof and floor, mainly due to poor compaction at the roof and the interaction with the highly permeable disturbed zone in the floor caused by the rock excavation technique.

In addition to these studies there is a project "Backfilling and closure of the deep repository" running. In this project the hydraulic conductivity of different backfill materials is investigated.

No experimental studies of transport of solutes in backfill materials have been done within the SKB program.

Table 3-8. Process/variable table for the process Advective transport of species.

Variable	Does this variable influence the process?		Does the process influence this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Temperature	Through viscosity	Effect is small and not considered in transport calculations	(Minor)	Through viscosity
Water content	(Yes)	See 3.2.1	No	
Gas content	Reduced flow in unsaturated clay	Advective transport of species during the unsaturated stage is not and issue	(Transport of dissolved gas)	Advective transport of dissolved gas is not an issue
Hydro-variables (pressure and flows)	Yes	Hydraulic conductivity is used to determine whether advection can occur	**Yes**	**Determines the advective flow**
Backfill geometry	Yes	Backfill dimensions are included in calculations	No	
Backfill pore geometry	Yes	Defines the hydraulic conductivity	(Yes)	See 3.2.1
Stress state	(Yes)	Swelling pressure is used to determine whether advection can occur	(Yes)	Through pore volume
Backfill composition	No		No	
Backfill pore water composition	Yes	Determines the hydraulic conductivity	Yes	Determines the exchange of species
Structural and stray materials	(Alternative transport paths)	Not considered in SR-Can – no route to alternative path has been found	No	

Natural analogues/observations in nature

No relevant observations have been made.

Time perspective

Advection in the backfill may occur at all timescales.

Handling in the safety assessment SR-Can

Advective transport of species in the tunnel backfill is included in the integrated modelling of the chemical evolution of the near field (Section 3.4.4).

Model: Radionuclide transport in the backfilled tunnels will be modelled by assuming transport controlled by advection-dispersion with sorption. The sorption coefficient will be based on the assumption of equilibrium sorption on the backfill material. As an alternative, transport dominated by diffusion into the backfill material with subsequent sorption on backfill material can be assumed.

Boundary conditions: The process is controlled by the hydraulic boundary conditions at the location in the repository.

Handling of variables influencing this process: All backfill properties and the hydraulic boundary conditions are included in the model. The effect of temperature is neglected.

Handling of variables influenced by the process: The mass transfer of species in the pore water is calculated.

Uncertainties

Uncertainties in mechanistic understanding

See Section 3.2.2 for uncertainties concerning water advective transport.

Model simplification uncertainties for the above handling in SR-Can

The uncertainty in the conceptualisation of radionuclide transport in tunnels can be regarded as fairly large as compared to the corresponding description in the rock. This is due to the fact that, at present, no experimental data exists to support the chosen concept. However, the advection-dispersion equation with equilibrium sorption is routinely utilised for describing solute transport in a porous medium such as a back-filled tunnel. The uncertainty thus does not stem from the concepts as such, but rather from the lack of site-specific experience within the SKB programme.

Input data and data uncertainties for the above handling in SR-Can

See Section 3.2.2 for uncertainties concerning water advective transport.

3.4.2 Diffusive transport of species

Overview/general description

An overview of diffusion processes and phenomena as relevant for the buffer is given in Section 2.5.3; these considerations also apply to a backfill consisting of bentonite/ballast or Friedland Clay.

The importance of these processes for the backfill materials considered here is difficult to quantify, because diffusion processes have not been studied in detail so far for either choice. It can generally be assumed that the EDL-effects on enhanced cation diffusion and anion exclusion will decrease with decreasing content of expandable 2:1 minerals and increasing pore size. In sand-bentonite mixtures EDL-effects are expected to be negligible (except at sufficiently high bentonite/sand ratios). In both types of proposed backfills, the content of smectite is about 20%, while a dry density of about 1,600 kg/m^3 (clay fraction) is envisaged in case of bentonite/rock and one of 1,780 kg/m^3 (bulk) in case of Friedland clay.

- Evidence from several different studies suggests that in case of material with a smectite content of about 95% to 45%, the overlap of EDLs leading to anion exclusion occurs at a dry density of about 1,200–1,500 kg/m^3 /Kozaki et al. 1998, Karnland 1997, Ochs et al. 2001/. The porosity of Kunigel-V1 at a dry density of 1,500 kg/m^3 is about 0.44. Apparent anion exclusion (expressed by an apparently smaller diffusion-available porosity for anions in comparison to HTO) has been found in natural clay formations with similar or even higher porosity (data for London and Boom clay quoted in /Nagra 2002/). Thus, it can be expected that this process can also be operative in Friedland clay under the foreseen conditions (porosity < 0.4).
- /Ochs et al. 2001/ found a similar effect of enhanced cation diffusion on D_e for Cs in the density range of about 1,800 – 800 kg/m^3 for MX-80 as well as Kunigel-V1 bentonite, which has a smectite content of about 45%. In case of Kunigel-V1 at a density of 800 kg/m^3, the bulk density of smectite will be about 360 kg/m^3, in comparison to about 320 kg/m^3 in case

of the foreseen bentonite/rock mixture. Therefore, it can be assumed that this process may also play a role for the diffusive transport in the backfill.

- /Sato 1998/ gives a comparison of effective diffusivities for HTO and anions (Cl, I) for Kunigel-V1 Na- bentonite (dry density: 1,600 kg/m^3) as a function of wt% sand added. The D_e values for both HTO as well as the anions increase by a factor of about 2–3 when the sand content is increased from 0 wt% to 70 wt%. This implies that under these conditions, anion exclusion was still operative in the bentonite/sand mixture. Assuming similar relations for MX-80 and the corresponding 30/70 bentonite/ballast mixture would result in D_e values similar to ones selected for Friedland Clay /Ochs 2005/. However, the influence of rock-derived ballast may be more significant than the influence of silica sand (cf /Pusch 1998/).
- Both enhanced cation diffusion and anion exclusion are further dependent on the ionic strength of the pore solution. High salinity depresses the EDL, thereby decreasing the importance of both processes.

Table 3-9. Process/variable table for the process Diffusive transport of species.

Variable	Does this variable influence the process?		Does the process influence this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Temperature	Yes	The temperature dependence of the diffusivity is not included in the transport calculations. The importance is regarded as small	No	
Water content	No (saturated conditions assumed)		No	
Gas content	No	(Saturated conditions assumed)	In case of dissolved gases such as CO2 or CH4	Diffusive transport of gases is considered
Hydro-variables (pressure and flows)	Saturated conditions assumed		No	
Backfill geometry	Yes	Backfill dimensions are included in calculations	No	
Backfill pore geometry	Yes	Defines the magnitude of the diffusivities	Possibly indirectly through influence on porewater composition and swelling	
Stress state	Indirectly through pore geometry		Possibly indirectly through influence on porewater composition and swelling	
Backfill composition	Through pore water composition	Defines the magnitude of the diffusivities	Indirectly through influence on porewater composition	
Backfill pore water composition	Extent of EDL depends on ionic strength	Defines the magnitude of the diffusivities	Through diffusive transport of main constituents	See 3.4.7
Structural and stray materials	(Through influence on physical pore width)	No stray materials within the backfill are considered	(Possibly indirectly through influence on porewater composition)	

Influence of temperature, porewater composition and speciation, pore geometry, sorption: Analogous to the relations discussed for the buffer in Section 2.5.3.

Influnce of backfill composition/density and structural/stray materials: To a first approximation, the additional non-expandable minerals present in the backfill are viewed as a dilution of the expandable clay fraction. This is consistent with observations on materials with different contents of expandable clay minerals (e.g. MX-80, Kunigel-V1, and Opalinus Clay, see above). The influence of soluble impurities on porewater composition is analogous to the buffer.

Influence on backfill variables: As pointed out in Section 2.5.5, the diffusion process is coupled to nearly all chemical processes through the diffusive transport of reactants. How chemical processes, such as exchange reactions of major ions, may further influence other backfill variables is discussed in Section 3.4.4.

Boundary conditions

The transfer of species from the buffer to the backfill can be visualised as the diffusion of dissolved species from the bentonite into a volume of similar clay with a lower density. The transfer of species from the backfill to the host rock can be visualised as the diffusion of dissolved species from the clay or bentonite/rock mixture into flowing water in the near-field fracture network (equivalent flow rate or Q_{eq}, see Section 2.5.3).

Model studies/experimental studies

While a large number of investigations are described in the literature concerning diffusion experiments in bentonite and similar smectite-rich clays (see /Yu and Neretnieks 1997/ for an overview), much less work has been done for natural clays poor in smectite and bentonite/ballast mixtures. Some data relevant for such materials are compiled in /Yu and Neretnieks 1997, Nagra 2002/, but no data are available for Friedland clay. Most diffusion studies are performed as transient in-diffusion experiments. These experiments yield D_a, which is a lump-sum representation of all processes relevant for radionuclide migration, including diffusion and sorption. This holds in particular for moderately and strongly sorbing radionuclides. Steady-state through-diffusion studies, which can yield De and porosity, are largely restricted to mobile tracers (Cs, HTO, anions). Few attempts have been made so far to derive diffusion coefficients through semi-mechanistic models. Some examples are discussed in Section 2.5.3 in the context of anion exclusion and enhanced cation diffusion.

Natural analogues/observations in nature

The usefulness of natural analogues for determining diffusion constants is limited due to the difficulty of determining what conditions existed in the past.

Time perspective

The process is active in all timescales, but is of less concern during the saturation phase.

Handling in the safety assessment SR-Can

Before saturation: The process is neglected since advection dominates.

After saturation: The process is included as a boundary condition in the scenario specific modelling of the backfill chemical evolution for the post-thermal long-term phase, see heading “Handling” for process 3.4.4. The process is treated in a simplified way with identical diffusivity for all elements.

Failed canister: Included in the modelling of radionuclide transport for the long-term phase, see heading "Handling" for process 2.5.3. For the treatment of radionuclide diffusion, element-specific effective diffusivities are used together with corresponding porosities (see Ochs 2005).

Boundary conditions: See sections referred to above.

Handling of variables influencing this process: Dependence on density, expected ionic charge of diffusing species, porewater composition and temperature is considered in the selection of diffusion constants for transport of radionuclides. For the treatment of diffusion within the backfill chemical evolution, see Section 3.4.4.

Uncertainties

Uncertainties in mechanistic understanding

Uncertainties in mechanistic understanding of diffusion in compacted, expandable clay materials are discussed in Section 2.5.3; this discussion applies also to the case of backfill. An additional uncertainty exists with regard to a mechanistic understanding of the effects of the large amounts of non-expandable minerals present in the candidate backfill materials.

Model simplification uncertainties for the above handling in SR-Can

As in the case of the buffer, diffusion is represented in a simplified way, through the use of selected constant effective diffusion coefficients and available porosities in the relevant transport codes (see Sections 3.4.4 and 2.6.1). In that sense, the diffusion input parameters have to be viewed as conditional; i.e. their application will only be valid under the conditions considered in data derivation. Therefore, uncertainties will be related to the selection of consistent conditions.

Input data and data uncertainties for the above handling in SR-Can

Input data to SR-Can are effective diffusivities and available porosities to be directly used in consequence calculations. Data and uncertainties for MX-80/rock are scaled directly from /Ochs and Talerico 2004/; the corresponding information for Friedland clay are given in /Ochs 2005/, from which data for consequence calculations are chosen in the SR-Can data report.

3.4.3 Sorption (including exchange of major ions)

Overview/general description

An overview of sorption and ion exchange processes as relevant for the buffer is given in Section 2.5.5; these considerations also apply to a backfill consisting of bentonite/ballast or Friedland Clay.

Montmorillonite is the principal mineral in bentonite and and an important component of the mixed layer montmorillonite/mica fraction of Friedland clay. Montmorillonite as well as mica are 2:1 layer silicates that consist of octahedral alumina sheets sandwiched between tetrahedral silica sheets. However, montmorillonite and mica differ in terms of layer charge and type of interlayer cation: Montmorillonite has a lower layer charge, with large hydrated cations (especially Na) occupying the interlayer space. This renders montmorillonite expandable, with a large interlayer surface area and high CEC. Micas possess a high layer charge compensated by K^+. The interlayer distance is small and the layers are not expandable. The surface area and CEC are therefore smaller than in case of montmorillonite. Both minerals feature the same two types of distinctly different types of surfaces (siloxane or "layer" surface and edges), where two main types of sorption take place /e.g. Sposito 1984, Stumm and Morgan 1996/.

The following table summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Table 3-10. Process/variable table for the process Sorption (including exchange of major ions).

Variable	Does this variable influence the process?		Does the process influence this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Temperature	Yes	Influence of temperature on sorption must be acknowledged, but effect is not clear	No	
Water content	Indirectly through porewater composition		No	
Gas content	Indirectly through porewater composition (CO2)		Possibly indirectly, through influence of Ca-exchange on carbonate equilibria	
Hydro-variables (pressure and flows)	Indirectly through porewater composition		Possibly indirectly, through porewater composition/ swelling	
Backfill geometry	No	(Total backfill mass considered)	No	
Backfill pore geometry	Possibly indirectly through influence on EDL properties		Possibly indirectly, through influence on EDL properties/ swelling	
Stress state	Indirectly through influence on porewater composition and EDL properties		Indirectly through influence on porewater composition and EDL properties	
Backfill composition	Yes	Chemical data used for sorption coefficient estimates	(Surface composition)	See 3.4.4
Backfill pore water composition	Yes	Chemical data used for sorption coefficient estimates	Yes	See 3.4.4
Structural and stray materials	Yes	Sorption on stray materials is conservatively excluded in SR-Can	Indirectly through influence on porewater composition and related mineral equilibria	

Influence of backfill and porewater composition, and of temperature: Analogous to the situation of the buffer (see Section 2.5.5).

Influence on backfill variables: The influence of ion exchange on the surface composition of layer silicates and on porewater composition is analogous to the situation of the buffer. The influence of these processes on pore geometry, and thereby on the hydraulic conductivity, is discussed in Section 3.3.1. Based on the data shown in Section 3.3.1, a significant difference between a 30/70 bentonite/ballast mixture and Friedland Clay can be expected. While the data in Figure 3-10 suggest that Friedland Clay compacted to the reference dry density of 1,780 kg/m^3 may behave in a similar way as the bentonite buffer, the data in Figure 3-9 suggest that conversion of the 30/70 bentonite/ballast mixture from the Na- to the Ca-form will cause a significant decrease of swelling pressure and corresponding increase in hydraulic conductivity.

Boundary conditions

Analogous to the situation of the buffer (see Section 2.5.5).

Model studies/experimental studies

Analogous to the situation of the buffer (see Section 2.5.5).

Time perspective

Analogous to the situation of the buffer (see Section 2.5.5).

Natural analogues/observations in nature

Analogous to the situation of the buffer (see Section 2.5.5).

Handling in the safety assessment SR-Can

Before saturation: The process is neglected.

After saturation: Ion exchange is included in the scenario specific modelling of the backfill chemical evolution for the thermal phase and the post-thermal long-term phase, see heading "Handling" for process 3.4.4.

Failed canister: Sorption is included in the modelling of radionuclide transport for the longterm phase, see heading "Handling" for process 3.3.15. As for the buffer, sorption is treated through element-specific K_d values derived for specific conditions (see /Ochs 2005/ for the definition of data and associated uncertainties).

Boundary conditions: See sections referred to above.

Handling of variables influencing this process: Dependence on the composition of the backfill and the corresponding porewater is considered in selecting K_d values for radionuclide transport. Because of the conditional nature of K_d, the data selected are derived for conditions expected to be relevant for PA calculations. Temperature effects are not considered explicitly, but the effects within the temperature range expected in the backfill are deemed to be covered with good margin by the uncertainties associated with the selected K_d values. For the influence of ion exchange and surface acid-base equilibria on the chemical evolution of the backfill, see Section 3.4.4; these processes are also taken into account in the derivation of radionuclide K_d values.

Uncertainties

Uncertainties in mechanistic understanding

The discussion given given for the buffer (Section 2.5.5) is also applicable to the backfill.

Model simplification uncertainties for the above handling in SR-Can

The data selection for the considered backfill materials is a direct extension of the approach taken for the buffer. The K_d concept for radionuclide transport modelling is basically justified under conditions far from surface saturation, which can be expected in the case of diffusion-limited radionuclide migration in a clay-based backfill. At the same time, K_d is a highly conditional parameter and has to be derived for each set of conditions. For the backfill this is done i) in case of the bentonite/ballast mixture by scaling the data derived for the bentonite buffer according to the respective proportion of smectite, and ii) in case of Friedland Clay by deriving the data directly for the specified conditions /Ochs 2005/. As pointed out in Section 2.5.5, use of a sorption model and direct use of recommended K_d values would lead to consistent results for the specified set of conditions (i.e. use of K_d would not introduce additional uncertainties, as long as the conditions remain constant). As long as the backfill material can be expected to represent a homogeneous geochemical compartment, no spatial variability needs to be taken into account.

Input data and data uncertainties for the above handling in SR-Can

Input data to SR-Can are K_d values to be directly used in consequence calculations. In case of a bentonite/ballast mixture, K_d values for radionuclide migration for various conditions, as well as the associated uncertainties are directly based on /Ochs and Talerico 2004/ by scaling for the smectite content. In case of Friedland clay, K_d values and uncertainties are derived separately for the relevant set of reference conditions /Ochs 2005/. The potential variability of K_d as a function of conditions is then evaluated in analogy to the results for bentonite.

3.4.4 Alterations of backfill impurities

Overview/general description

The backfill material consists not only of montmorillonite, but also other accessory minerals as well as impurities. In the repository environment, these can be dissolved and sometimes re-precipitated depending on the prevailing conditions.

Basically, the same chemical processes that occur in the buffer may also act in the backfill (Section 2.5.6).

The main differences are:

1. The temperature in the backfill much lower and the thermal gradients are small. Dissolution/precipitation of minerals due to temperature effects is of minor importance in the backfill.
2. The initial composition is different. This is not very important for the 30/70 mixture, since the clay component is identical to the buffer material. Friedland clay does contain other minerals.
3. Both advective and diffusive transport of species may be active in the backfill.

Table 3-11 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Boundary conditions

There are no particular boundary conditions to discuss for these processes. The relevant boundary conditions in order to treat the process quantitatively are those of the transport processes that control the exchange of solutes between the tunnel backfill water and the water in its adjacent components, i.e. the boundary conditions of the processes diffusion and advection.

For alterations of impurities, the exchange of a number of solutes like sodium and calcium ions, carbonate and molecular oxygen is relevant.

Model studies/experimental studies

No specific studies of chemical processes in the backfill have been done prior to SR-Can. Some of the work done with buffer materials is of relevance for the backfill as well (Section 2.5.6).

Natural analogues/observations in nature

Some of the work done for buffer materials may be of relevance for the backfill as well (Section 2.5.6).

Table 3-11. Process/variable table for the process Alterations of backfill impurities.

Variable	Does this variable influence the process?		Does the process influence this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Temperature	Temperature highly influences the extent of precipitation/dissolution of secondary minerals.	Minor effect since the temperature increase in the backfill is small	No	
Water content	Yes, could affect concentrations	However, the chemical model assumes saturated conditions	No	
Gas content	A secondary effect from water content variations.		Yes	Dissolved gases are included in the model
Hydro-variables (pressure and flows)	Yes	Darcy flow is included in the model	No	
Backfill geometry	Yes	(Total backfill mass considered)	No	
Backfill pore geometry	Yes	Determines the diffusivity see 3.4.2	Precipitation-dissolution of minerals	Included in model but of minor concern in backfill
Stress state	Yes	Partial pressures are included in model	Yes	The results from the model is evaluated to consider effects on swelling pressure
Backfill composition	Yes	Composition data is considered in model	Yes	The evolution of the composition is calculated with the model
Backfill pore water composition	Yes	Composition data is considered in model	Yes	The evolution of the composition is calculated with the model
Structural and stray materials	Yes	See 3.4.7	Secondary mineral formation/dissolution may influence the alteration of structural components. This is particularly true for sulphates.	The fate of structural material is not evaluated in SR-Can

Time perspective

All timescales.

Handling in the safety assessment SR-Can

Before saturation: Geochemical processes will be the same both before and after saturation phases. This is just a matter of water flow and solutes transport.

Thermal period: The thermal effects on the chemical evolution of the backfill are not included in SR-Can, since the temperature elevation and the thermal gradiens are small.

After saturation: The process is included in the scenario specific modelling of the buffer chemical evolution for post-thermal long-term phase. The model considers advection, diffusion, ion-excange and mineral dissolution/precipitation in the backfill compartment. Figure 3-12 shows an example from the modelling of the pH evolution in the backfill. pH in the backfill is

Figure 3-12. *Example of the pH evolution in the backfill.*

buffered by calcite precipitation-dissolution, which in turn is affected by calcium availability due to cation exchange processes. As exchange reactions reach the equilibrium with incoming water more easily in the backfill than in the buffer (where the CEC is larger), the excess of calcium is used to precipitate calcite until equilibrium, decreasing the pH of pore water in the backfill.

Failed canister: In the case of a failed canister, vast amounts of metallic iron, originating from the corroding cast iron canister insert, will be added to the geochemical system. This will be included in the model mentioned above, in a dedicated calculation case.

Boundary conditions: Main model: The diffusive transfer of species between the flowing water and the bentonite is explicitly modelled. The near-field evolution model uses the Qeq concept to handle the boundary conditions. This is sufficient to estimate a general timescale on which the evolution occurs.

Handling of variables influencing this process: The modelling is in itself a coupling of the four (groups of) processes mentioned above and is thus a coupled modelling of most of the significant long-term chemical processes. A large number of the variable influences related to the chemical conditions (pore water composition, montmorillonite composition, bentonite composition) are also included.

Handling of variables influenced by the process: The geochemical conditions in the nearfield as a function of time and space will be calculated.

The changes in the buffer accessory mineral content as a consequence of the thermal stage has been modelled, but not validated through a comparison with experimental and/or natural analogue data. This makes it difficult to ensure that changes due to the thermal stage are minor or that these results should be assumed to be the initial conditions for the low temperature stage.

In addition to the processes discussed above, the behaviour of silica and clay minerals and their effect on cementation could be addressed by performing some scoping calculations considering the present knowledge on kinetic dissolution-precipitation of smectite, silica-phases and the precipitation of alternative clay minerals (kaolinite and/or illite). These scoping calculations would give some qualitative information on the relative importance of these processes and the effect on bentonite properties, i.e. porosity changes. See also Section 2.5.9.

Uncertainties

Uncertainties in mechanistic understanding

Some critical uncertainties remain concerning the mechanistic understanding of the processes that control the redox state of the bentonite system. It is not clear yet to which extent pyrite and/or siderite are the main redox controlling phases, although either process, or their combination, will scavenge the remaining oxygen in the near field. This should be discerned by comparative modelling of pyrite and siderite kinetic availability.

In addition, most of the secondary precipitation/dissolution processes that are temperature driven are thermodynamically controlled. Hence, there is no need for a detailed mechanistic understanding. However, some of the silicate transformations are kinetically controlled and their mechanistic understanding in compacted bentonite conditions is poor. This is mainly related to clay mineral transformations (dissolution of smectite and precipitation of illite and/or kaolinite). Although these reactions occur at a very slow rate, their effect on the overall geochemical evolution is not yet clear.

Finally, it is assumed that pH is buffered by the equilibrium with calcite. However, the amount (or even the presence) of this mineral phase is somewhat uncertain, depending on the bentonite type selected as backfill component, thus the pH buffering capacity of the backfill could be affected.

Model simplification uncertainties for the above handling in SR-Can

Secondary dissolution and precipitation processes have not been fully implemented in a coupled model of backfill evolution. The processes are only considered when required for the definition of critical master variables in the system (pH and pe). A possibility could be to couple the THM processes occurring with the key chemical processes that will control the geochemical evolution of the backfill system.

There are a number of accessory minerals, such as silicates other than silica, which are not included in the models, as most of them tend to dissolve at a very slow kinetic rate. Other silicates (usually clay minerals) precipitate at similarly slow rates. However, the dissolution-precipitation processes involving these two groups of minerals could affect the stability of montmorillonite as well as the chemical composition of the backfill pore water, thus affecting the chemical long-term evolution of the bentonite. See also Section 2.5.9.

There is no model accounting for the dissolution/precipitation of accessory minerals during the water saturation stage of the backfill. As water flux will be faster than when the backfill is water saturated and the bentonite composition will be far from equilibrium with incoming water, some changes will occur faster. These changes will account for step compositional gradients in the backfill and changes in porosity as accessory minerals dissolve and/or precipitate, leading to changes in hydraulic properties of the backfill. Thus, modelling of the system must therefore be coupled to the THM processes that proceed in parallel with transport and chemical reactions. A submodel dealing with the saturation stage of the backfill will, at least, give an idea on the magnitude of theses changes.

As there is some uncertainty associated to the accessory mineral content of the bentonite component, especially for those minerals that can play a significant role on the pH and/or redox buffering capacity of the backfill, the model will consider variable amounts of these minerals, even their absence from the intial accessory mineral pool. Thus the effect of dissolution/precipitation of these minerals on the master variables could be assessed.

Input data and data uncertainties for the above handling in SR-Can

Key thermodynamic data are well established and therefore reliable. The main uncertainties remain in the definition of the kinetically controlled processes. These are linked to the mechanistic uncertainties previously mentioned.

Proper data for surface reactions (i.e. cation exchange and edge site reactions) is of paramount importance for the correct assessment of the bentonite behaviour. Two types of information are needed for geochemical modelling: i) Cation occupancy of the CEC and protonation state of the smectite surface, and ii) Exchange and protonation-deprotonation constants. The main uncertainty associated with these data is related to the experimental conditions used for their determination (i.e. low bentonite density and high solid/liquid ratios). Recent experiments have addressed this problem, however there is still a large uncertainty related to the determination of cation exchange constants and their variation as a function of bentonite density. These data and the associated uncertainties will tentatively be handled in the SR-Can data report.

3.4.5 Aqueous speciation and reactions

This process is in general identical with the same process for the buffer (Section 2.5.7)

3.4.6 Osmosis

Overview/general description

The general principle for this process is the same as for the corresponding buffer process (Section 2.5.8). The absolute effects of osmosis increases with increasing montmorillonite/water ratio, but swelling pressure increases more, and the relative pressure drop is consequently more pronounced at low montmorillonite/water ratios. The tunnel backfill material is consequently more sensitive to osmosis if the montmorillonite/water ratio is lower than in the buffer, which is the case in the bentonite/crushed rock material. On the other hand, if the backfill consolidation properties are based on swelling pressure, i.e. if the backfill has a high enough clay water ratio, then the osmotic effect will be similar to that of the buffer. Figure 3-13 shows measured swelling pressure for various concentrations of sodium and calcium chloride groundwater versus clay dry density for the reference bentonite Deponit CaN (Milos) and MX-80 (Wyoming). Both clays have been purified from accessory minerals and ion exchanged into pure sodium and calcium state, respectively. The calcium exchanged clays were exposed to calcium chloride solutions and the sodium exchanged clays to sodium chloride solution. It is obvious that the two clays react very similar to the exposure to salt solutions. The measured osmotic effects are well in accordance with the ion-equilibrium theory both with respect to concentrations and type of cation.

The cation exchange capacity (CEC) of the Friedland bulk material is around 0.25 eq/kg, which is approximately one third that of the high quality Milos and Wyoming bentonites /Karnland et al. 2006/. The clay fraction has a CEC of around 0.45 eq/kg, and the active clay mineral is a mixed layer illite/smectite with approximately one third illite layers. The resulting sealing properties are therefore significantly different at the same bulk density (Figure 3-14, left). The clay mineralogical differences compared to MX-80 and Deponit CaN lead to less god sealing properties also at the same ratio between water mass and clay mass, i.e. also if the amount of accessory minerals is compensated for. Consequently, the Friedland material has to be compacted to a significantly higher clay density, compared to the MX-80 and Deponit CaN clays, in order to reach the same sealing effect.

At relatively high densities, corresponding to short distances between the clay mineral flakes, the swelling pressure is due to a crystalline and an osmotic effect. There is no general consensus concerning the exact cause and quantification of the crystalline component, but hydration of cations and of the mineral surfaces plays an important role. The relative effect of the crystalline component increases at increasing clay density, i.e. at decreasing distance between mineral flakes. Concequently, the osmotic component in the Friedland clay will be smaller, compared to the Wyoming and Milos clays at the same swelling pressure. Theoretically this leads to

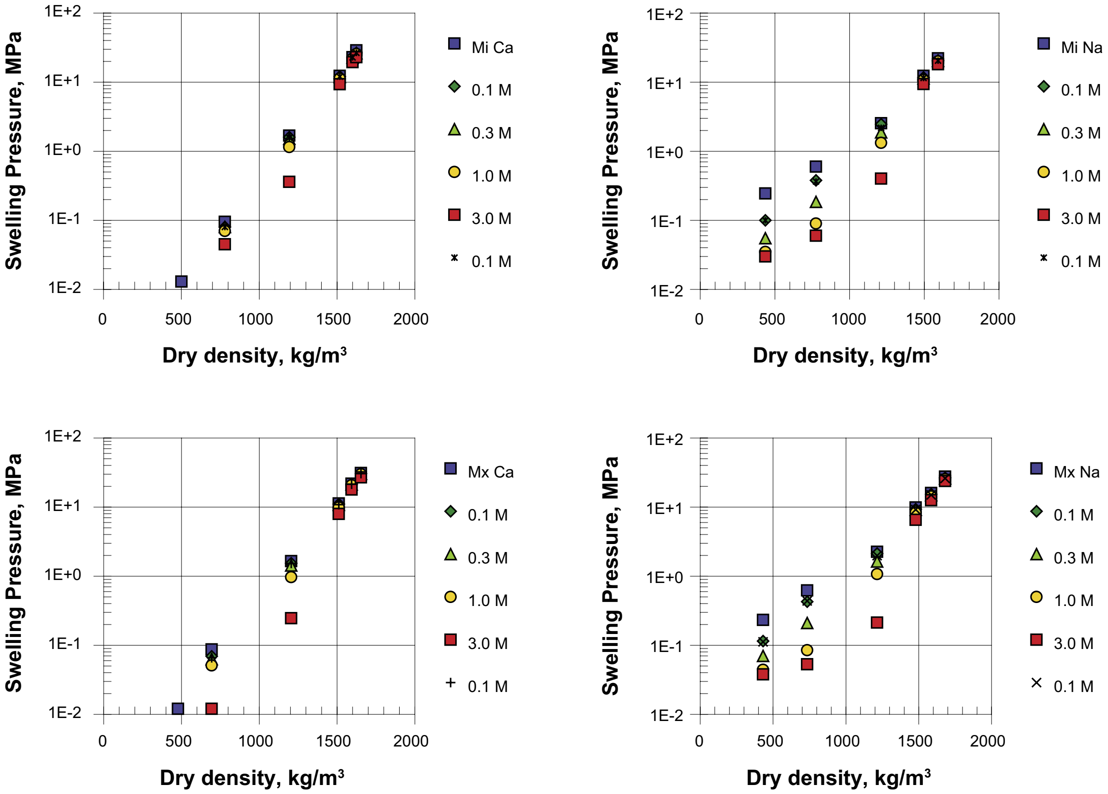

Figure 3-13. Measured swelling pressure in purified and homo-ionic Deponit CaN (upper) and MX-80 (lower) for calcium conditions (left) and sodium conditions (right). Figures indicate solution concentration in moles/L for calcium chloride in calcium exchanged samples sodium chloride in the sodium exchanged samples, respectively.

different ion equilibrium conditions in the two clays at equilibrium with salt groundwater, resulting in a smaller pressure reduction in the Friedland clay. Figure 3-14 right shows swelling pressure measured in the Friedland and Wyoming clays, which are in equilibrium with different concentrations of external NaCl solutions. The measured pressures are plotted versus swelling pressure at pure water conditions in order to facilitate the comparison. Note that the clay density is higher in the Friedland clay at the same pressure. The measured reductions in the Friedland clay are approximately half the reduction in the MX-80 clay, which is in agreement with modelling results.

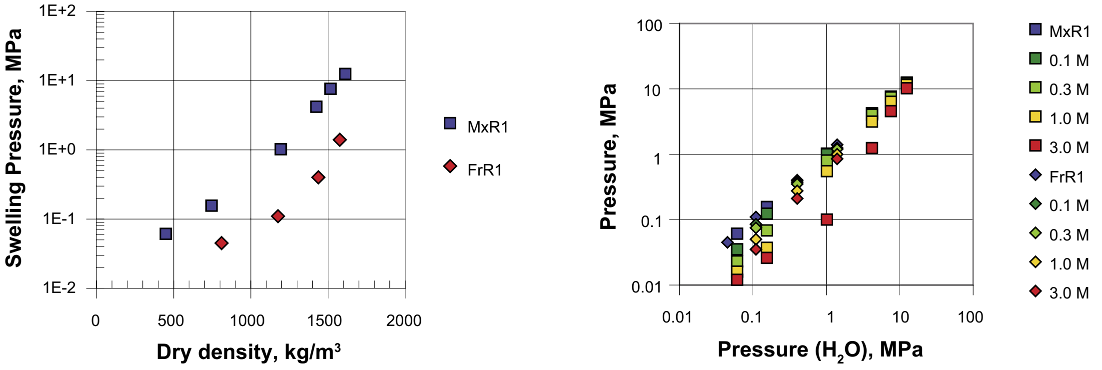

Figure 3-14. Left: swelling pressure at fresh water conditions for the MX-80 (MxR1) and the Friedland (FrR1) clays versus clay density. Right: Measured swelling pressure in MX-80 (MxR1) and Friedland (FrR1) clays versus measured measured pressure at pure water conditions. Figures indicate NaCl concentration in moles/L.

Table 3-12 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Boundary conditions

The boundary conditions are the cation concentration and cation valence of the groundwater in contact with the tunnel backfill.

Model studies/experimental studies

The studies reported in the buffer section are relevant also for the tunnel backfill (Section 2.5.8).

Natural analogues/observations in nature

The study reported in the buffer section is relevant also for the tunnel backfill (Section 2.5.8).

Table 3-12. Process/variable table for the process Osmosis.

Variable	**Does this variable influence the process?**		**Does the process influences this variable?**	
	Influence present?	**Handling of influence?**	**Influence present?**	**Handling of influence?**
Temperature	Minor	Ignored	No	
Water content	Increasing water content makes the relative effects increase	Saturated condition assumed	Only at extreme conditions where dehydration may occur	Not within the range of SR-Can waters
Gas content	No		No	
Hydrovariables (pressure and flows)	Affects the water activity and thereby the chemical potential	Minor effect which is not considered	Important effect on hydraulic conductivity	Effects of salinity on hydraulic conductivity are evaluated
Backfill geometry	No		Only at extreme conditions where dehydration may occur	Not within the range of SR-Can waters
Backfill pore geometry	Interlayer distance is a decisive parameter	Indirect via composition	Rearrangement of pore sizes at extreme conditions	Not within the range of SR-Can waters
Stress state	The swelling pressure is related to ion ditribution	Indirect via composition	Reduction of swelling pressure	Effects of salinity on swelling pressure are evaluated
Backfill composition	The content and structure of the montmorillonite part is decisive. The charge compensating cation in the montmorillonite is of importance	Included in assessment of hydraulic conductivity and swelling pressure	No	
Backfill pore water composition	Of decisive importance	Effects of salinity on swelling pressure and hydraulic conductivity	Governs the interlayer ion concentration and thereby likely transport properties	Only effects on the backfill properties are considered
Structural and stray materials	No		No	

Time perspective

The process is relevant for all time perspective in the lifetime of a repository. The effect of a change in groundwater salinity is expected to result in an almost instantaneous response in swelling pressure.

Handling in the safety assessment SR-Can

The effects of the ionic strength of the groundwater on the hydraulic properties of the backfill are handled by direct application of empirical data.

Time periods:

Resaturation/thermal period and period up to first glaciation: The hydraulic conductivity and swelling pressure of the backfill are estimated based on the groundwater composition at the site.

Glacial cycle: The hydraulic conductivity and swelling pressure of the backfill are estimated based on the evolution of the groundwater composition.

Handling of variables influencing this process: The montmorillonite composition and the groundwater/porewater composition are directly included in the model.

Handling of variables influenced by the process: The backfill swelling pressure and hydraulic conductivity will be calculated.

Boundary conditions: The composition of the groundwater in the repository.

The special cases of failed canister and of earthquakes: Will not affect this process

Uncertainties

Same as for buffer (Section 2.5.8).

3.4.7 Montmorillonite transformation

Overview/general description

The general principle for this process is the same as for the corresponding buffer process (Section 2.5.9). In principle all possible transformation processes are very temperature dependent. The temperature is significantly lower in the tunnel backfill compared to the buffer, and transformation processes in the backfill is consequently even less probable compared to in the buffer. One possible exception is pH dependant local alteration in volumes that are in direct contact with concrete, e.g. tunnel plugs or wall reinforcement.

Table 3-13 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Boundary conditions

See buffer section (Section 2.5.9).

Model studies/experimental studies

The studies reported in the buffer section are relevant also for the tunnel backfill (Section 2.5.9).

Table 3-13. Process/variable table for the process Montmorillonite transformation.

Variable	Does this variable influence the process?		Does the process influences this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Temperature	Yes	Included in transformation expression	No	
Water content	Reduced transformation in unsaturated clay	No credit taken	At extreme tranformation	
Gas content	No		No	
Hydrovariables (pressure and flows)	Supply of water (potentially harmful species)	Included in transformation evaluation	Indirect through Bentonite composition	Effect on hydraulic conductivity is evaluated
Backfill geometry	Amount of buffer	Included in evaluation	At extreme transformation	–
Backfill pore geometry	Indirect through Bentonite composition		Indirect through Bentonite composition	
Stress state	No		Yes	Loss of swelling is evaluated
Backfill composition	Yes	Included in transformation expression	Yes	Included in transformation expression
Backfill pore water composition	Harmful species	Included in transformation expression	(Yes) to a small extent	**Only effects on the buffer itself are considered**
Structural and stray materials	Amount and type of cement	Assumed "safe" in SR-Can	No	

Natural analogues/observations in nature

The studies reported in the buffer section are relevant also for the tunnel backfill (Section 2.5.9).

Time perspective

Significant transformation is not expected during the lifetime of the repository according to the kinetic model for illitization.

Handling in the safety assessment SR-Can

The alteration of the swelling component in the backfill is treated the same way as for the buffer (Section 2.5.9). The only difference is the maximum temperature and the amount of material.

Uncertainties

Same as for the buffer (Section 2.5.9).

3.4.8 Colloid release

Overview/general description

Water uptake by the tunnel backfill material and its resultant swelling is limited by the tunnel walls, and a swelling pressure is developed in the backfill material. Fractures intersecting the tunnel imply that no swelling restrictions are present, and that swelling continues until a thermodynamic equilibrium is reached without the development of swelling pressure. This free swelling may lead to separation of individual montmorillonite layers, or small groups of mineral layers (dispersion).

A principal difference between the tunnel backfill material and the buffer is obvious. Colloid release from the buffer leads to replacement of lost montmorillonite by swelling of the remaining montmorillonite, which leads to a slow lowering of the buffer density. In principle, the buffer material will thereby stay relatively homogeneous and the sealing properties will decrease generally but very slowly. In contrast to the situation in the buffer, the remaining accessory minerals in the backfill may serve as a filter and prevent replacement of lost material. This potential filter effect will reduce the loss of montmorillonite, but it may lead to high local hydraulic conductivity in the depleted part of the backfill. The grain size distribution of the accessory material will determine the extent of such a filter function.

Table 3-14 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Boundary conditions

The boundary conditions are the cation concentration and cation valence of the groundwater in contact with the outermost part of the tunnel backfill.

Model studies/experimental studies

All studies reported in the buffer section are relevant also for the tunnel backfill (Section 2.5.10).

Table 3-14. Process/variable table for the process Colloid release.

Variable	Does this variable influence the process?		Does the process influences this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Temperature	Negligible		No	
Water content	Indirect through stress state		No	
Gas content	No		No	
Hydrovariables (pressure and flows)	May determine the rate of colloid release	Included in current model	Indirect through backfill geometry	
Backfill geometry	Amount of backfill present	Included in evaluation	backfill loss	Included in evaluation
Backfill pore geometry	No		No	
Stress state	Yes		Indirect through buffer geometry	
Backfill composition	Impurities in the backfill may have an effect	Included in current model – to a certain extent – not fully understood	(Selective loss of the clay component)	
Backfill pore water composition	Only occurs if [M2+] < 0.001 M		Colloid source	Only effects on the backfill itself are considered
Structural and stray materials	No		No	

Natural analogues/observations in nature

All studies reported in the buffer section are relevant also for the tunnel backfill (Section 2.5.10).

Time perspective

Colloid release is only possible at very low ion concentrations and likely only relevant in conjunction with a glaciation. The effects will be significant only in the long-term perspective. However, local effects around the periphery of the material are possible, and the time perspective is thereby shorter than in the buffer.

Handling in the safety assessment SR-Can

Same as for the buffer (Section 2.5.10).

Uncertainties

Same as for the buffer (Section 2.5.10).

3.4.9 Radiation-induced transformations

Overview/general description

Montmorillonite in the backfill can be broken down by γ radiation. The result is a decrease in the montmorillonite concentration. The process can be neglected in the backfill based on the same reasoning as for the buffer (Section 2.5.11).

3.4.10 Microbial processes

Overview/general description

Micro-organisms interact with their surroundings, and they commonly have a significant effect on the geochemical record of their environment. From a microbiological perspective, the backfill environment will constitute an environment with mixed characters from two other well defined environments of the repository concept; the geosphere and the buffer. This backfill environment will, however, have some characteristics that significantly distinguish it from the two other mentioned environments. One is the possible presence of organic material in structural and stray material. Another is the gas/water interface that will develop during the saturation process. Finally, there will be oxygen in the backfill until it has been consumed and reduced by microbes and/or by inorganic oxygen scavengers such as sulphides.

The effects of microbial processes on the chemical stability of the geosphere have been thoroughly discussed elsewhere in this report (ref. Geosphere-microbial processes). Similar effects can be obtained in the backfill, but the differences in the variables “structural and stray materials, the temperature, and the gas content” compared to the geosphere may increase the rates of microbial processes during an initial phase that is relatively short compared to the expected lifetime of the repository.

Microbial processes in the buffer have also been discussed elsewhere in this report (2.5.13). Those processes are expected to be limited to an initial phase, after which temperature, radiation, desiccation and the swelling pressure will sterilise the buffer /Pedersen 2002/. The radiation, desiccation and the swelling pressure effects on microbial processes in the backfill will be less pronounced and continued microbial activity will be possible.

Table 3-15 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Can.

Boundary conditions

The access to organic material, e.g. stray materials and methane and electron acceptors (ref Table 5-6 in SR-CAN geosphere) will set the limits for microbial process rates in the backfill.

Table 3-15. Process/variable table for the process Microbial processes.

Variable	Does this variable influence the process?		Does the process influence this variable?	
	Influence present?	Handling of influence?	Influence present?	Handling of influence?
Temperature	Most microbes have an ideal temperature range in which they thrive. Maximum temperature for life is 113°C.	Microbial effects in the backfill is not considered in SR-Can	No	
Water content	Water is needed for active life.	Microbial effects in the backfill is not considered in SR-Can	No	
Gas content	Hydrogen and methane can be consumed by microbes that will grow and produce biomass; largest effect is obtained if oxygen is present.	Microbial effects in the backfill is not considered in SR-Can	Microbes both produce and consume gases	Microbial effects in the backfill is not considered in SR-Can
Hydro-variables (pressure and flows)	No		No	
Backfill geometry	No		No	
Backfill pore geometry	No		Growth of microbes generate biomass that may clog pores	Microbial effects in the backfill is not considered in SR-Can
Stress state	No		No	
Backfill composition	No		No	
Backfill pore water composition	Microbes are sensitive to the geochemical situation, and may utilise pore water components for growth	Microbial effects in the backfill is not considered in SR-Can	Microbial activity may change the composition, e.g. by consumption of methane, sulphate and organic carbon and production of sulphide and carbon dioxide	Microbial effects in the backfill is not considered in SR-Can
Structural and stray materials	Organic parts of this material may be a food source for microbes with growth as the result.	Microbial effects in the backfill is not considered in SR-Can	Microbes may oxidise organic components in this material.	Microbial effects in the backfill is not considered in SR-Can

Model studies/experimental studies

The ongoing backfill experiment at Äspö hard rock laboratory includes microbial investigations. Large amounts of different micro-organisms were added locally to positions in the backfill. At decommission the survival and activity of added as well as naturally occurring microbes in the backfill will be analysed.

In addition, analysis of gas in the gas phase in the prototype repository at Äspö HRL and micro-organisms in the groundwater around the prototype repository have been performed /Pedersen 2004/. There was not water in the repository at the time of sampling for microbiological analysis. However, as soon as the prototype is approaching saturation, such analysis is doable. The results showed presence of micro-organisms in the groundwater and demonstrated that groundwater gases such as methane and hydrogen have increased significantly in concentration in the gas phase since closure.

Natural analogues/observations in nature

No natural analogues or observations are known.

Time perspective

The time perspective concerning survival and activity of microbes in backfill have been summarized in a conceptual model as follows /confer Figure 3-5 in Pedersen 2000c/. At the time of deposition there will be backfill, possibly structural and other stray materials and an oxygenated gas phase in the tunnels. The first event will be filling of the void gas volume with groundwater. Microbes will be present in the water and these microbes will mix with the backfill. As the backfill will have some organic material from the bentonite, and possibly structural and stray material at local spots along the tunnel walls and floor, microbial activity will start soon. Methane will also intrude. As long as oxygen is present, rapid microbial oxidation of methane and organic material will turn the backfill environment to a reduced and anaerobic environment, which is beneficial for the repository. This is a process that will commence as soon as groundwater enters the backfill. Oxygen will probably disappear within weeks in the groundwater. Pockets with oxygen in a gas phase may stay oxygenised for longer times. But as soon as oxygen diffuses into the water, where microbes are active, it will be consumed and reduced. The risk for oxygenic copper corrosion will consequently rapidly diminish as a result of microbial processes.

Handling in the safety assessment SR-Can

Mass balance calculations can be made to show how different kinds of residual materials remaining in the repository will contribute to microbial oxygen reduction. It can be assumed that all organic matter will be able to serve as nutrients for microbes. Furthermore, the availability of hydrogen will be decisive for microbial activity in the long term. This means that an increased effect of microbial activity must be expected until all organic matter has been consumed, and subsequently an activity that is controlled by the supply of hydrogen will proceed. This means that oxygen, ferric iron, sulphate and carbon dioxide will be reduced to water, ferrous iron, sulphide and methane, respectively. The scope of these reactions is dependent on mass flows.

Uncertainties

Uncertainties in mechanistic understanding

The knowledge about microbial processes in the backfill is not yet well supported by experimental data. Rather, the processes are inferred from research on microbial processes in the geosphere and the buffer.

Model simplification uncertainties

Not relevant since a model for microbial processes in the backfill is lacking (compare with 2.5.13).

Input data and data uncertainties

Not relevant since a model for microbial processes in the backfill is lacking (compare with 2.5.13).

3.4.11 Speciation of radionuclides

See buffer Section 2.5.14.

3.4.12 Transport of radionuclides in water phase

See buffer Section 2.6.1.

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