

Technical Report

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Buffer, backfill and closure process report for the safety assessment SR-Site

Svensk Kärnbränslehantering AB

November 2010

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Update notice

The original report, dated November 2010, was found to contain both factual and editorial errors which have been corrected in this updated version. The corrected factual errors are presented below.

Updated 2014-01

Location	Original text	Corrected text
Page 121, Paragraph 3 from the end	Similarly, /Bradbury and Baeyens 1997/	Similarly, /Baeyens and Bradbury 1997/
Page 352, Paragraph 4 from the end, Reference Bradbury Baeyens 1997	Bradbury M H, Baeyens B, 1997. A mechanistic description of Ni and Zn sorption on Na-montmorillonite. Part II: Sorption experiments, J. Contaminant Hydrology, 27, 223-248.	Baeyens B, Bradbury M H, 1997. A mechanistic description of Ni and Zn sorption on Na-montmorillonite. Part I: Titration and Sorption Measurements. Journal of Contaminant Hydrology, 27, pp 199-222.
Page 365, Reference Sandén T, Börgesson L, 2010	Deep repository – engineered barrier system. Early effect of water inflow into a deposition hole. Laboratory test results. SKB Report in preparation.	Early effects of water inflow into a deposition hole. Laboratory test results. SKB R-10-70, Svensk Kärnbränslehantering AB.

Updated 2011-09

Location	Original text	Corrected text
Page 21, Table 2-4, Table title		New text added last in the table header. White fields (in the earthquake column) denotes processes where the authors have been unable to judge the significance of the process.
Page 21, Table 2-4, Row Bu5, column "long term"	10 ¹² m/s	10 ⁻¹² m/s
Page 21, Table 2-4, Row Bu7, column Long-term	Bu17	Bu18
Page 22, Table 2-4, Row Bu15, column Resaturation	System model (initial swelling)	Evaluation through comparison with empirical data.
Page 22, Table 2-4, Row Bu16, kolumn Earthquakes	Part of the integrated treatment buffer/canister/rock	Part of integrated assessment of buffer/canister/rock. (Mark the box red)
Page 22, Table 2-4, Row Bu17, column Long-term	Only considered for defective canister: Included in a separate scenario	Only considered for failed canister. Possible loss of buffer efficiency.
Page 28, Table 2-9, Row BfT18, column 3	Yellow	Red
Page 28, Table 2-9, Row BfT21, kolumn Resaturation	Analytic	<i>Text deleted</i>
Page 31, Table 2-12, Processes for tunnel plugs		Row Pg8 deleted (table renumbered)
Page 118, Table 3-12, Row Porewater composition	RN-transport model (section 3.5.6) and geochemical model (section 3.6.2).	RN-transport model (section 3.6.2) and geochemical model (section 3.5.6).
Page 150, Table 3-17, Row Pore geometry, column 3	<i>No text</i>	Included in model/expression used
Page 150, Table 3-17, Row Montmorillonite composition, column 3	<i>No text</i>	Included in model/expression used
Page 165, Table 3-23, Row Bentonite composition, column 3	<i>No text</i>	Neglected since the effect is very small
Page 179, Table 3-27, Row buffer geometry	See 1.3.3	See 3.3.3

Location	Original text	Corrected text
Page 211, Table 4-9, Row Backfill porewater composition	See 3.4.7	See 4.4.4
Page 224, Table 4-13, Row Backfill pore geometry	<i>No text</i>	Included in transformation evaluation
Page 224, Table 4-13, Row Stress state, last column	Loss of swelling can be evaluated	Loss of swelling is evaluated as a case with a high conductivity backfill
Page 225, Table 4-14, Row Stress state, column 3	<i>No text</i>	Included in modelling
Page 227, Table 4-15, Row Backfill pore geometry	<i>No text</i>	Neglected due to limited amounts of organic carbon
Page 227, Table 4-15, Row Gas content, column 5	<i>No text</i>	Neglected, since gas in the backfill is of limited concern
Page 227, Table 4-15, Row Hydrovariables, column 5	<i>No text</i>	Neglected, since extent is limited
Page 235, Table 5-2, Row Plug materials, column 5	See erosion	See Section 5.2.4
Page 235, Table 5-2, Row Porewater composition, column 5	Section 5.6	Section 5.4
Page 237, Table 5.3, Row Pore geometry, column 5	See erosion	See Section 5.2.4
Page 237, Table 5.3, Row Plug materials, column 5	<i>No text</i>	Neglected, since extent is limited
Page 246, Table 5-7, Row Porewater composition, column 5	<i>No text</i>	Included in modelling
Page 251, Table 5.8, Row water content, column 2, 3, 4	<i>No text</i>	Column 2: Yes, availability of water Column 3: Saturated conditions assumed Column 4: No
Page 251, Table 5.8, Row Gas content, column 2, 3, 4	<i>No text</i>	Column 2: Indirectly through water content Column 3: blanc Column 4: No
Page 281, Table 6-9, Row Structural and stray materials, column 5	<i>No text</i>	Neglected
Page 303, Table 7-5, column 5	No text in six rows	Neglected inserted in six rows
Page 303, heading first paragraph	Handling in the safety assessment SR-Can	Handling in the safety assessment SR-Site
Page 328, Table 8-8	Two rows missing Water content and gas content	Water content and Gas content inserted
Page 334, Table 9-1, Row Gas content, column 3	...the buffer will be...	...the bentonite will be...
Page 339, Table 9-3, Row Borehole geometry, column 4	...the buffer swell...	...the bentonite swell...
Page 339, Table 9-3, Row Pore geometry, column 4	...the buffer swell...	...the bentonite swell...
Page 344, Table 9-5, Row Pore geometry, column 5	<i>No text</i>	Included in model

Preface

This report gives an account of how processes in buffer, deposition tunnel backfill and the closure important for the long-term evolution of a KBS-3 repository for spent nuclear fuel, will be documented in the safety assessment SR-Site.

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 in collaboration with the concerned experts. Patrik Sellin has edited the report.

This report has been reviewed by Geert Volckert, SCK-CEN, David Read, Enterpris ltd and Esther Jonsson SKB according to the instructions for the SR-Site project. The reviewers' comments with answers will be made available as project documentation.

Stockholm, November, 2010

Allan Hedin

Project leader, SR-Site

Contents

1	Introduction	9
1.1	Role of this report in the SR-Site assessment	9
1.1.1	Overall methodology	9
1.1.2	Identification of processes	11
1.1.3	Relation to specific sites	12
1.1.4	Intended audience of this report	12
1.2	Structure for process descriptions	12
1.3	Participating experts	14
1.4	Handling of FEP's mapped to the buffer, backfill and closure process system	15
2	Definition of system components and summary of handling of processes in SR-Site	17
2.1	Overview	17
2.2	Buffer	17
2.2.1	Initial state of the buffer	17
2.2.2	Definition of buffer variables	18
2.2.3	Buffer performance and safety	19
2.2.4	Summary of handling of buffer processes in SR-Site	20
2.3	Backfill	24
2.3.1	Initial state of the backfill in SR-Site	24
2.3.2	Definition of backfill variables	25
2.3.3	Backfill performance	25
2.3.4	Summary of handling of backfill processes in SR-Site	26
2.4	Tunnel plug	28
2.4.1	Initial state of the tunnel plug	28
2.4.2	Definition of tunnel plug variables	30
2.4.3	Summary of handling of tunnel plug processes in SR-Site	31
2.5	Central area	32
2.5.1	Initial state of the central area	32
2.5.2	Definition of central area variables	32
2.5.3	Summary of handling of central area processes in SR-Site	34
2.6	Top Seal	35
2.6.1	Initial state of the top seal	35
2.6.2	Definition of top seal variables	35
2.6.3	Summary of handling of top seal processes in SR-Site	36
2.7	Bottom plate	38
2.7.1	Initial state of the bottom plate	38
2.7.2	Definition of bottom plate variables	38
2.7.3	Summary of handling of bottom plate processes in SR-Site	39
2.8	Borehole seals	40
2.8.1	Initial state of the borehole seals	40
2.8.2	Definition of variables for borehole seals	42
2.8.3	Summary of handling of borehole seal processes in SR-Site	42
3	Processes in the buffer	45
3.1	Radiation-related processes	45
3.1.1	Radiation attenuation/heat generation	45
3.2	Thermal processes	47
3.2.1	Heat transport	47
3.2.2	Freezing	52
3.3	Hydraulic processes	57
3.3.1	Water transport under unsaturated conditions	57
3.3.2	Water transport under saturated conditions	66
3.3.3	Gas transport/dissolution	71
3.3.4	Piping/Erosion	80
3.4	Mechanical processes	85
3.4.1	Swelling/mass redistribution	85
3.4.2	Liquefaction	103

3.5	Chemical processes	103
3.5.1	Introduction	103
3.5.2	Advective transport of species	105
3.5.3	Diffusive transport of species	107
3.5.4	Colloid transport	114
3.5.5	Sorption (including ion-exchange of major ions)	117
3.5.6	Alterations of impurities	124
3.5.7	Aqueous speciation and reactions	133
3.5.8	Osmosis	135
3.5.9	Montmorillonite transformation	139
3.5.10	Iron – bentonite interaction	148
3.5.11	Montmorillonite colloid release	151
3.5.12	Radiation-induced transformations	160
3.5.13	Radiolysis of porewater	162
3.5.14	Microbial processes	164
3.5.15	Cementation	171
3.6	Radionuclide transport processes	174
3.6.1	Speciation of radionuclides	174
3.6.2	Transport of radionuclides in the water phase	175
3.6.3	Transport of radionuclides in a gas phase	178
4	Processes in the tunnel backfill	181
4.1	Thermal processes	181
4.1.1	Heat transport	181
4.1.2	Freezing	184
4.2	Hydraulic processes	186
4.2.1	Water uptake and transport under unsaturated conditions	186
4.2.2	Water transport under saturated conditions	192
4.2.3	Gas transport/dissolution	197
4.2.4	Piping/erosion	199
4.3	Mechanical processes	201
4.3.1	Swelling/mass redistribution	201
4.3.2	Liquefaction	207
4.4	Chemical Processes	207
4.4.1	Advective transport of species	207
4.4.2	Diffusive transport of species	209
4.4.3	Sorption (including exchange of major ions)	213
4.4.4	Alterations of backfill impurities	215
4.4.5	Aqueous speciation and reactions	221
4.4.6	Osmosis	221
4.4.7	Montmorillonite transformation	223
4.4.8	Backfill colloid release	224
4.4.9	Radiation-induced transformations	226
4.4.10	Microbial processes	226
4.5	Radionuclide transport processes	229
4.5.1	Speciation of radionuclides	229
4.5.2	Transport of radionuclides in the water phase	229
5	Processes in the tunnel plugs	231
5.1	Thermal processes	231
5.1.1	Heat transport	231
5.1.2	Freezing	233
5.2	Hydraulic processes	234
5.2.1	Water uptake and transport under unsaturated conditions	234
5.2.2	Water transport under saturated conditions	236
5.2.3	Gas transport/dissolution	238
5.2.4	Piping/erosion	238
5.3	Mechanical processes	240
5.3.1	Swelling/mass redistribution	240
5.4	Chemical processes	242

5.4.1	Advection	242
5.4.2	Diffusive transport of species	244
5.4.3	Sorption (including exchange of major ions)	244
5.4.4	Alteration of concrete	245
5.4.5	Aqueous speciation and reactions	250
5.4.6	Osmosis	250
5.4.7	Montmorillonite transformation	250
5.4.8	Montmorillonite colloid release	250
5.4.9	Microbial processes	250
5.5	Radionuclide transport processes	253
5.5.1	Speciation of radionuclides	253
5.5.2	Transport of radionuclides in the water phase	253
5.5.3	Transport of radionuclides in a gas phase	253
6	Processes in the central area	255
6.1	Thermal processes	255
6.1.1	Heat transport	255
6.1.2	Freezing	258
6.2	Hydraulic processes	260
6.2.1	Water uptake and transport under unsaturated conditions	260
6.2.2	Water transport under saturated conditions	266
6.2.3	Gas transport/ dissolution	268
6.2.4	Piping/erosion	269
6.3	Mechanical processes	271
6.3.1	Swelling/mass redistribution	271
6.3.2	Liquefaction	275
6.4	Chemical Processes	275
6.4.1	Advective transport of species	275
6.4.2	Diffusive transport of species	277
6.4.3	Sorption	277
6.4.4	Alteration of the central area backfill	280
6.4.5	Alteration of concrete components	285
6.4.6	Aqueous speciation and reactions	285
6.4.7	Osmosis	285
6.4.8	Corrosion of steel components	285
6.4.9	Microbial processes	286
6.4.10	Colloid release	288
6.4.11	Radiation induced transformation	288
6.5	Radionuclide transport processes	288
6.5.1	Speciation of radionuclides	288
6.5.2	Transport of radionuclides in the water phase	289
7	Processes in the top seal	291
7.1	Thermal processes	291
7.1.1	Heat transport	291
7.1.2	Freezing	291
7.2	Hydraulic processes	293
7.2.1	Water uptake and transport under unsaturated conditions	293
7.2.2	Water transport under saturated conditions	296
7.2.3	Gas transport/dissolution	297
7.2.4	Piping/erosion	298
7.3	Mechanical processes	298
7.3.1	Swelling/mass redistribution	298
7.3.2	Liquefaction	301
7.4	Chemical Processes	302
7.4.1	Advective transport of species	302
7.4.2	Diffusive transport of species	303
7.4.3	Sorption (including exchange of major ions)	304
7.4.4	Alteration of concrete components	305
7.4.5	Aqueous speciation and reactions	306

7.4.6	Colloid release	306
7.4.7	Steel corrosion	306
7.4.8	Microbial processes	306
7.4.9	Radiation induced transformation	307
7.5	Radionuclide transport processes	307
7.5.1	Speciation of radionuclides	307
7.5.2	Transport of radionuclides in the water phase	307
8	Processes in the bottom plate	309
8.1	Thermal processes	309
8.1.1	Heat transport	309
8.1.2	Freezing	312
8.2	Hydraulic processes	312
8.2.1	Water uptake and transport under unsaturated conditions	312
8.2.2	Water transport under saturated conditions	314
8.2.3	Gas transport/dissolution	316
8.2.4	Piping/erosion	317
8.3	Mechanical processes	317
8.3.1	Swelling/mass redistribution	317
8.3.2	Liquefaction	320
8.4	Chemical processes	320
8.4.1	Advective transport of species	320
8.4.2	Diffusive transport of species	322
8.4.3	Sorption (including exchange of major ions)	324
8.4.4	Alteration of concrete	327
8.4.5	Aqueous speciation and reactions	327
8.4.6	Corrosion of copper	327
8.4.7	Microbial processes	327
8.5	Radionuclide transport processes	329
8.5.1	Speciation of radionuclides	329
8.5.2	Transport of radionuclides in the water phase	329
9	Processes in borehole seals	333
9.1	Thermal processes	333
9.1.1	Heat transport	333
9.1.2	Freezing	333
9.2	Hydraulic processes	335
9.2.1	Water uptake and transport under unsaturated conditions	335
9.2.2	Water transport under saturated conditions	338
9.2.3	Gas transport/dissolution	340
9.2.4	Piping/erosion	340
9.3	Mechanical processes	340
9.3.1	Swelling/mass redistribution	340
9.3.2	Liquefaction	343
9.4	Chemical processes	343
9.4.1	Advective transport of species	343
9.4.2	Diffusive transport of species	345
9.4.3	Sorption (including exchange of major ions)	347
9.4.4	Alteration of concrete	347
9.4.5	Aqueous speciation and reactions	347
9.4.6	Copper corrosion	347
9.4.7	Alteration of impurities in bentonite	348
9.4.8	Osmosis	348
9.4.9	Montmorillonite transformation	348
9.4.10	Montmorillonite colloid release	348
9.4.11	Microbial processes	349
9.5	Radionuclide transport processes	349
9.5.1	Speciation of radionuclides	349
9.5.2	Transport of radionuclides in the water phase	349
10	References	351

1 Introduction

1.1 Role of this report in the SR-Site assessment

1.1.1 Overall methodology

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

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

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

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

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

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

2. Description of the initial state.

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

3. Description of external conditions.

Factors related to external conditions are handled in the categories "climate-related issues", "large-scale geological processes and effects" and "future human actions". The handling of climate-related issues is described in the SR-Site Climate report /SKB 2010h/, whereas the few external, large-scale geosphere processes are addressed here in the Geosphere process report /SKB 2010i/. The treatment of future human actions in SR-Site is described in the SR-Site FHA report /SKB 2010j/.

4. Compilation of process reports.

The identification of relevant processes is based on earlier assessments and FEP screening. All processes identified 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 2010k/ and for the geosphere /SKB 2010i/. Also short-term geosphere processes/alterations, due to repository excavation, are included. For each process, its general characteristics, the time frame in which it is important, the other processes to which it is coupled and how the process is handled in the safety assessment are documented.

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

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

6. Compilation of input data.

Data to be used in the quantification of repository evolution and in dose calculations are selected. The process of selection and the data adopted are reported in a dedicated Data report /SKB 2010/. 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 isolation potential of the system over time is analysed, yielding a description of the general system evolution and an evaluation of the safety function indicators. Each process is handled in accordance with the plans outlined in the process reports. Radiological consequences of potential canister failures are not analysed in this step.

8. Selection of scenarios.

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

9. Analysis of scenarios.

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

10. Additional analyses.

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

11. Conclusions.

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

This Buffer, Backfill and Closure process report is one of the process reports required to complete step 4. The purpose of the process reports is to document the scientific knowledge of the processes to a level required for their adequate treatment in the safety assessment. The documentation is not exhaustive from a scientific point of view, since such a treatment is neither necessary for the purposes of the safety assessment nor possible within the scope of an assessment. However, it must be sufficiently detailed to facilitate, by arguments founded on scientific understanding, the treatment of each process

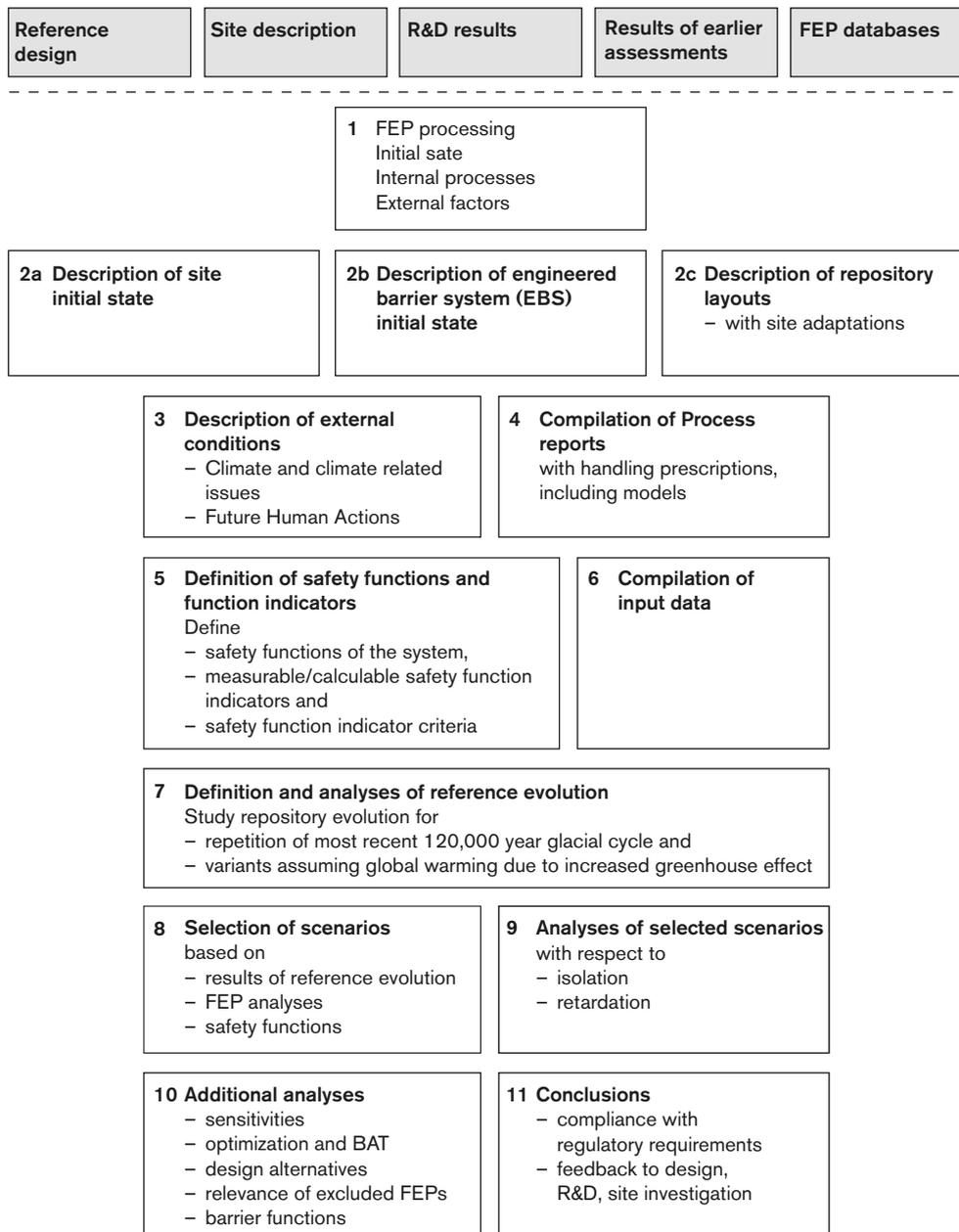


Figure 1-1. An outline of the eleven main steps of the SR-Site safety assessment. The boxes above the dashed line are inputs to the assessment.

in the safety assessment. The purpose is to determine how to handle each process in the safety assessment at an appropriate degree of detail, and to demonstrate how uncertainties are taken care of, given the suggested handling. The means of handling processes established in this report are used in the analysis of the reference evolution, step 7, and in the analyses of scenarios, step 9.

1.1.2 Identification of processes

The process documentation in this SR-Site process report is an update and extension of the descriptions in the SR-Can version of the Process report /SKB 2006a/. The extension concerns processes for the system components not treated in detail in SR-Can, i.e. tunnel plugs, central area, top seal, bottom plate in deposition holes and borehole seals. The SR-Can version of the report, in turn, builds on the process documentation in the SR 97 version of the process report /SKB 1999/ and the FEP processing carried out in SR-Can. The complementary FEP processing carried out in SR-Site (step 1 above) did not identify any need to modify the list of relevant processes that were included in the SR-Can version of the process

report /SKB 2006a/, see the SR-Site FEP report /SKB 2010a/ for details. However, some modifications have been made to improve the structure and logic of the process descriptions. For example, to improve the clarity of the documentation and the handling of uncertainties in the geochemical evolution of the buffer, some mechanisms included in integrated descriptions in SR-Can are included as separate processes in SR-Site, e.g. iron-bentonite interactions and cementation. For the system components not treated in detail in SR-Can, the list of processes has been established largely based on those defined for the buffer and backfill. A complete list of processes described in the SR-Site process reports can be found in the abovementioned FEP report.

1.1.3 Relation to specific sites

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

1.1.4 Intended audience of this report

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

1.2 Structure for process descriptions

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

Overview/general description

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

Dependencies between process and system variables

For each system component, in this case the buffer, backfill, tunnel plugs, central area, top seal, bottom plate in deposition holes and borehole seals, a set of physical variables that defines the state of the system is specified. For each process, a table is presented under this heading with documentation of how the process is influenced by the specified set of physical variables and vice versa, i.e. how the process influences the variables. In addition, the handling of each influence in SR-Site is indicated in the table.

Boundary conditions

The boundary conditions for each process are discussed. These refer to the boundaries of the buffer, backfill, tunnel plugs, central area, top seal, bottom plate in deposition holes and borehole seal systems, respectively. The processes for which boundary conditions need to be described are, in general, related to transport of material or energy across the boundaries.

Model studies/experimental studies

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

Time perspective

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

Natural analogues/observations in nature

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

Handling in the safety assessment SR-Site

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

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

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

Boundary conditions: The handling of boundary conditions is discussed, especially any spatial and temporally varying chemical and hydraulic conditions.

Influences and coupling to other processes: The handling of the documented influences is discussed, as is coupling to other processes within that part of the system.

The method of treatment for all processes is discussed and where relevant,, the models that have been developed for each process are described.

Handling of uncertainties in SR-Site

The handling of different types of uncertainties associated with each process is summarised.

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

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

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

Adequacy of references supporting the handling in SR-Site

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

References

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

1.3 Participating experts

The experts involved in assembling the basic information on the processes are listed in Table 1-1. All these experts are included in the SR-Site list of experts as required by the SR-Site QA plan , see further the SR-Site Main report /SKB 2011/.

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

Process	Expert author, affiliation
Radiation attenuation/heat generation	Patrik Sellin, SKB
Heat transport	Harald Hökmark, Clay Technology
Freezing	Martin Birgersson, Clay Technology
Water uptake and transport for unsaturated conditions	Lennart Börgesson Clay Technology
Water transport for saturated conditions	Lennart Börgesson 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
Advective transport of species	Ola Karnland, Clay Technology
Diffusive transport transport of species	Michael Ochs, BMG
Sorption (including ion-exchange)	Michael Ochs, BMG
Alterations of impurities	David Arcos, Amphos XXI
Aqueous speciation and reactions	Patrik Sellin, SKB
Osmosis	Ola Karnland, Clay Technology
Montmorillonite transformation	Ola Karnland, Clay Technology
Iron-bentonite interaction	Daniel Svensson, SKB
Montmorillonite colloid release	Magnus Hedström, Clay Technology
Radiation-induced transformations	Patrik Sellin, SKB
Radiolysis of porewater	Patrik Sellin, SKB
Microbial processes	Karsten Pedersen, University of Göteborg
Cementation	Ola Karnland, Clay Technology
Colloid transport	Patrik Sellin, SKB
Speciation of radionuclides	Patrik Sellin, SKB
Transport of radionuclides in water phase	Patrik Sellin, SKB
Transport of radionuclides in gas phase	Patrik Sellin, SKB
Copper corrosion	Patrik Sellin, SKB
Steel corrosion	Patrik Sellin, SKB
Concrete degradation	David Arcos, Amphos XXI

1.4 Handling of FEP's mapped to the buffer, backfill and closure process system

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

As mentioned above, the complementary FEP processing has not led to any revision of the list of buffer and backfill processes compared with those treated in the previous SR-Can assessment. For the system components not treated in detail in SR-Can, i.e. tunnel plugs, central area, top seal, bottom plate in deposition holes and borehole seals, it was found appropriate to establish the list of processes based on those defined for the buffer and backfill.

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

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

2 Definition of system components and summary of handling of processes in SR-Site

2.1 Overview

This section defines and describes the system components and gives a summary of their handling in the SR-Site safety assessment. The components have been defined as:

- Buffer
- Backfill
- Tunnel plug
- Central area
- Top seal
- Bottom plate
- Bore hole seals

In describing the production and installation of the components in the Production reports /SKB2010d, e, f, g/ that also serve as supporting documentation for SR-Site, slightly different definitions have been used. The **Backfill Production Report** /SKB2010e/ covers the backfill and the tunnel plugs, the **Closure Production Report** /SKB2010f/ covers the central area, top seal and bore hole seals and the bottom plate is included in the Underground openings construction report /SKB2010g/. The title of this report is based on the titles of the production reports.

2.2 Buffer

2.2.1 Initial state of the buffer

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 Buffer Production Report /SKB 2010d/. A specified set of variables, see Section 2.2.2, is used to describe the buffer.

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-Site. One is a natural Na-bentonite of Wyoming type (MX-80) supplied by the American Colloid Company and the other is IBECO RWC (also called 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.

MX-80 contains accessory minerals in addition to smectite: albite, quartz, cristobalite, muscovite and gypsum, and also, grains of pyrite, calcite, siderite, barite and iron hydroxides (see Table 2-1). The mean chemical composition, as analysed by ICP/AES, of MX-80 expressed as oxides is: 57% SiO₂, 18.5% Al₂O₃, 3.6% Fe₂O₃, 2.3% MgO, 1.3% CaO, 2.0% Na₂O, 0.5% K₂O, 0.2% TiO₂, 0.3% total carbon, 0.3% total sulphur, and 13.7% loss of ignition.

Minerals other than smectite in Milos-bentonite are mainly calcite, dolomite, quartz, and cristobalite, see Table 2-1. The mean chemical composition, expressed as oxides as analysed by ICP/AES, of the bentonite is 48% SiO₂, 15.7% Al₂O₃, 4.56% Fe₂O₃, 2.92% MgO, 5.4% CaO, 0.7% Na₂O, 0.8% K₂O, 0.7% TiO₂, 1.0% total carbon, 0.7% total sulphur, and 20% loss of ignition.

There are primarily two methods available for fabricating bentonite blocks and rings; uniaxial pressing and isostatic pressing. Here is assumed that all blocks will be manufactured by uniaxial pressing.

Table 2-1. Composition of MX-80 and Deponit CA-N bentonite including, impurities and accessory minerals in /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%
Ca ²⁺	18%	46%	5%
Mg ²⁺	8%	29%	5%
K ⁺	2%	2%	1%

The bentonite, bought in bulk form and transported by ship, is subject to quality control both before loading onto the ship and at reception. This is done to ensure that the quality is within the specifications and that there is no contamination during transport. Quality control is also undertaken during manufacture of the blocks and rings; one important check is the water content before pressing so that this can be adjusted to obtain 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/m³. The bulk density is dependent on the gaps left between the canister and buffer and between buffer and rock. The gaps are a results of the space needed to install the blocks. The slot between the canister tube and the buffer is 10 mm wide and the slot along the circumferential boundary between the buffer and the rock is 50 mm in the Buffer Production Report/SKB 2010d/. The slots are filled with bentonite pellets.

Buffer emplacement in the deposition holes 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. The buffer is put into position by a specially designed buffer filling vehicle. The buffer positioning is thereafter checked and adjusted if necessary. The emplacement of the copper canister is done with a specially designed deposition machine. A top bentonite block is installed immediately after the canister is emplaced with the buffer installation equipment. The final handling procedures and the final design of the buffer installation equipment and the deposition machine have not yet been decided, 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 buffer must be protected from water or high humidity until the tunnel is backfilled. The reason is that the buffer may start swelling before deposition of the canister and before the tunnel backfill 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 temporary rubber protection sheet that is kept sealed until backfilling of the tunnel starts. The temporary rubber protection sheet and drain tube would be removed after use.

2.2.2 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 interface with the rock surface of the deposition hole, at the bottom by an interface with the copper plate on top of the concrete plate at the base of the borehole and on the top by its interface with the backfill.

The buffer is characterised thermally by its temperature distribution 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, sometimes by gas content (desaturation) and by hydrovariables (pressure and flows), which are mainly of interest in the transient period when the buffer is being saturated with water.

The buffer is characterised mechanically by its stress state.

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

The variables are defined in Table 2-2. The values of some of the variables are dependent on the density of the different phases. The following values have been used: density of water (ρ_w) 1,000 kg/m³ and density of clay solids (ρ_{cs}) 2,780 kg/m³.

The initial values of the variables, i.e. the values at the time of deposition, are given in the Buffer Production Report /SKB 2010d/.

2.2.3 Buffer performance and safety

In order to evaluate buffer performance in the safety assessment, a number of so called function indicators have been formulated together with criteria that these should fulfil over time, see further the SR-Site main report, /SKB 2011/. The criteria are summarised in Table 2-3, with reference to the sections in this report where the criteria are discussed. Some of the criteria does not directly relate to buffer properties (e.g. temperature).

The content of canister corroding agents in the buffer should be low. Apart from unavoidable initial amounts of oxygen, the pyrite content could pose a long-term problem, as pyrite, if not oxidised by initially present or intruding oxygen, will release sulphide, a canister corroding agent. There is, however, no absolute criterion placed on this amount.

Table 2-2. 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 in buffer as a function of time and space. The total 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 content (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.
Montmorillonite composition	The mean molecular structure of montmorillonite including the type of charge compensating cations.
Porewater composition	Composition of the porewater (including any radionuclides and dissolved gases) in time and space in the buffer.
Structural and stray materials	Chemical composition and quantity of any stray materials accidentally left in the buffer. At this stage, no structural materials are defined for this component.

Table 2-3. 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	3.3.2
Swelling pressure	> 1 MPa	Ensure tightness, self sealing	3.4.1
Maximum temperature ¹	$T^{Buffer} < 100^{\circ}\text{C}$	Ensure that the buffer will retain its favourable properties in the long term	3.5.9
Minimum temperature	$T^{Buffer} > -4^{\circ}\text{C}$	Avoid freezing	3.2.2
Swelling pressure around entire canister	> 0.2 MPa	Avoid canister sinking (criterion to be determined)	3.4.1
Buffer saturated density around entire canister	> 1,800 kg/m ³	Reduce microbial activity	3.5.14
Buffer saturated density around entire canister	> 1,650 kg/m ³	Prevent colloid transport through buffer	3.5.4
Buffer density around entire canister	< 2,050 kg/m ³	Ensure protection of canister against rock shear	3.4.1

Several characteristics of the groundwater composition are essential for providing chemically favourable conditions for the repository. These are discussed in the **Geosphere Process Report /SKB 2010i/**, but some of them are directly related to the performance of the buffer:

- The salinity of the groundwater should neither be too high, nor too low. The total charge concentration of cations should exceed 4 mM in order to avoid colloid release from buffer and backfill, hence: $\Sigma q[M^{q+}]^{GW} > 4$ mM (Section 3.5.11). Groundwaters of high ionic strengths would have a negative impact on the buffer properties (Section 3.5.8) In general, ionic strengths corresponding to NaCl concentrations of around 100 g/L (1.7 M NaCl) is tolerable for the buffer, but no specific criterion is given.
- Regarding pH, a criterion can be formulated from the point of view of buffer and backfill stability $\text{pH} < 11$ (Section 3.5.9). This is fulfilled for any natural groundwater in Sweden. However, construction and stray materials in the repository, in particular concrete, could contaminate the groundwater such that high pH values are reached.

2.2.4 Summary of handling of buffer processes in SR-Site

Table 2-4 summarises the handling of buffer processes in the safety assessment SR-Site, as suggested in this report. In the table, the process is either “mapped” to a model by which it will be quantified or, alternatively a brief verbal description of how it will be handled is provided. Since the initial evolution, characterised by unsaturated conditions and elevated temperatures, is in many respects different from the long-term, saturated period, 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 evaluation of the final result of the swelling for a number of input data combinations, including osmotic effects due to intruding saline water.

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 affected to any significant extent by the thermal and unsaturated conditions and are therefore neglected during the early saturation and thermal phases. One typical example would be the process “freezing”.

Table 2-4. 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. White fields (in the earthquake column) denotes processes where the authors have been unable to judge the significance of the process.

	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 > -4°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)
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 Bu18	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 in an unsaturated material	Neglected since liquefaction from a short pulse cannot occur in a high density bentonite, due to high effective stresses	Neglected since liquefaction from a short pulse cannot occur in a high density bentonite, due to high effective stresses	
Bu10 Advective transport of species	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"

	Resaturation/ "thermal" period	Long-term after saturation and "thermal" period	Earthquakes	Notes
Bu11 Diffusive transport transport of species	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	Not specifically treated	
Bu13 Alteration of impurities	Chemistry model (thermal, saturated phase; unsaturated phase disregarded)	Chemistry model	Not specifically treated	
Bu14 Aqueous speciation and reactions	Chemistry model (thermal, saturated phase; unsaturated phase disregarded)	Chemistry model	Not specifically treated	
Bu15 Osmosis	Evaluation through comparison with empirical data.	Evaluation through comparison with empirical data	Not specifically treated	Handling of long-term intrusion of saline water
Bu16 Montmorillonite transformation	Model calculations (thermal, saturated phase; unsaturated phase disregarded)	Estimate based on evidence from nature	Part of integrated assessment of buffer/canister/rock	
Bu17 Iron-bentonite interaction	Neglected since no iron will be in contact with the bentonite	Only considered for failed canister. Possible loss of buffer efficiency	Only considered for failed canister. Possible loss of buffer efficiency	
Bu18 Montmorillonite colloid release	Neglected if total cation charge is > 4 mM. Otherwise modelled	Neglected if total cation charge is > 4 mM. Otherwise modelled	Not specifically treated	Loss of buffer mass is calculated See also water transport under saturated conditions
Bu19 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	Neglected since dose rate outside canister is too low to have any effect	
Bu20 Radiolysis of porewater	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	Neglected since dose rate outside canister is too low to have any effect	
Bu21 Microbial processes	Neglected under unsaturated conditions, since the extent of aqueous reactions is limited. For saturated condi- tions the treatment is the same as for "Long-term"	Quantitative estimate of sulphate reduction, limited by supply of microbe nutrients in groundwater	Not specifically treated	
Bu22 Cementation	Discussed together with Process Bu16 "Montmorillonite transformation"	Discussed together with Process Bu16 "Montmorillonite transformation"	Part of integrated assessment of buffer/canister/rock	

	Resaturation/ "thermal" period	Long-term after saturation and "thermal" period	Earthquakes	Notes
Failed canister				
Bu6 Failed canister. Gas transport/ dissolution	Quantitative estimate based on empirical data (<i>no failures are expected this period</i>)	Quantitative estimate based on empirical data	Quantitative estimate based on empirical data	
Bu19 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 from a failed canister is estimated	The effect of α -radiation from nuclides is estimated in Section 2.5.11. There, it is concluded that the consequences can be neglected.
Bu23 Colloid transport	Neglected if density at saturation > 1,650 kg/m ³ , otherwise bounding calculation (<i>no failures are expected this period</i>)	Neglected if density at saturation > 1,650 kg/m ³ , otherwise bounding calculation	Neglected if density at saturation > 1,650 kg/m ³ , otherwise bounding calculation	
Bu24 Speciation of radionuclides	No failures are expected this period	Assumptions based on empirical data	Assumptions based on empirical data	
Bu25 Transport of radio- nuclides in water phase	No failures are expected this period	COMP23	COMP23 Reduced diffusion path	
Bu26 Transport of radionuclides in gas phase	No failures are expected this period	Quantitative estimate	Quantitative estimate	

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 intrusion of dilute groundwater during glacial conditions must be addressed if the hydrogeochemical analyses imply that ionic strengths below the given criterion (Section 3.5.11) cannot be excluded. Colloidal release needs to be modelled accordingly.

The effects of chemical evolution on key properties such as 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 taking into account radionuclide speciation, necessary for the selection of diffusion and sorption data and 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 potential dose consequences is estimated by a bounding calculation case.

2.3 Backfill

2.3.1 Initial state of the backfill in SR-Site

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-Site Production line report for backfill /SKB 2010e/. 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. In SR-Site, the deposition tunnels as well as the transport tunnels and the lower part of the ramp and shaft, extending from 200 m down to the repository is assumed to be filled with backfill material and will be considered as “backfill”.

One backfill concept will be analysed in SR-Site:

- Precompacted blocks of a natural swelling clay (not necessarily a bentonite), IBECO-RWC-BF (manufacturer’s name) or Milos-B (SKB term) bentonite is used as an example of such a material in SR-Site. The entire tunnel is filled with pre-compacted blocks. The gaps between the rock and the blocks are filled with pellets of the same material. An example of the block filling is given in Figure 2-1. The backfilling in the top part of the deposition hole is shown in Figure 2-2. The estimated volumes and proposed densities are given in Table 2-5.

The choice of IBECO-RWC-BF is based on a large number of tests /Gunnarsson et al. 2006/ which showed that the material together with a feasible backfilling technique fulfils the requirements with an acceptable margin. The composition of IBECO-RWC-BF is given in Table 2-6.

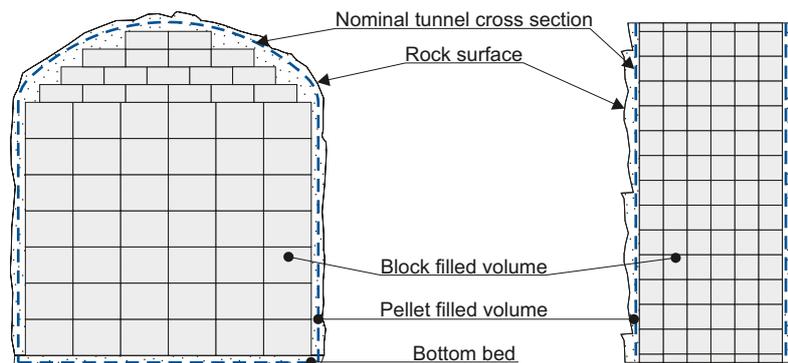


Figure 2-1. Example of block configuration in a fictive tunnel section /SKB 2010e/.

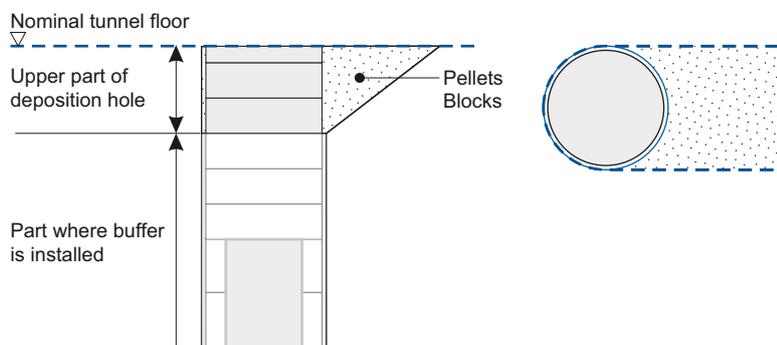


Figure 2-2. Backfill in the top section of the deposition hole /SKB 2010e/.

Table 2-5. Calculated installed dry density for the reference design of backfill components and installed backfill. The tunnel volume is set to the largest acceptable. From the Backfill Production Report /SKB 2010e/.

Parameter	Tunnel cross section	Upper part of deposition hole
Dry density of blocks (ρ_{db})	1,700 kg/m ³	1,710 kg/m ³
Dry density of pellets (ρ_{dp}) ¹	1,000 kg/m ³	1,200 kg/m ³
Volume fraction of slots between blocks (dV_s)	2%	0
Volume of pellets filling and bottom bed	Total volume minus block and void part of the volume Nominal: 25–16,8*(1+0.02) m ³ /m Accepted: 25–0.60*25(1+0.02) m ³ /m	2.56 m ³
Total volume	Maximum allowed tunnel blasting volume 25 m ³ /m	5.17 m ³
Calculated installed dry density (nominal block part of cross section and largest acceptable tunnel volume)	1,458 kg/m ³	1,457 kg/m ³
Calculated installed dry density (acceptable block part of cross section and largest acceptable tunnel volume)	1,408 kg/m ³	–

For the tunnel cross section the same density is used for the pellets filling between blocks and tunnel walls and bottom bed.

Table 2-6. Composition of IBECO RWC-BF.

Component	Reference design (wt-%)	Accepted variation
Montmorillonite	50–60%	45–90%
Dominant exchangeable cation	Ca	Na
CEC (meq/100g)	75	> 60

2.3.2 Definition of backfill variables

The deposition tunnels are 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 2010e/, the subsystem is constrained also by the rock around rejected deposition holes.

The transport tunnels are constrained by the surrounding rock as well as tunnel plugs separating them from the deposition tunnels and the central area.

The backfill in the tunnels 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 is also defined by the porewater composition and the occurrence of structural and stray materials in the deposition tunnel.

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 2-7.

The initial values of the variables are given in the Backfill Production Report /SKB 2010e/.

2.3.3 Backfill performance

In order to evaluate the performance of the tunnel backfill, a few so called function indicators have been established together with criteria these should fulfil over time, see further the SR-Site main report. These criteria are summarised in Table 2-8, referencing sections in this report where the reasoning for these criteria are given.

Table 2-7. 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 total 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 content (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	Total chemical composition and content of the backfill material (including any radionuclides) in time and space.
Backfill porewater composition	Composition of the porewater (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 2-8. 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	4.2.2
Swelling pressure	$P_{Swell}^{Backfill} > 0.1$ MPa	Ensure homogeneity and avoid preferential pathways	4.3.1
Minimum temperature	$T^{Backfill} > -2^{\circ}\text{C}$	Avoid freezing	4.1.2

2.3.4 Summary of handling of backfill processes in SR-Site

Table 2-9 summaries the handling of backfill processes in the safety assessment SR-Site, as suggested in this report. In the table, the process is either “mapped” to a model by which it will be quantified or a brief verbal description of how it will be handled is provided. 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 saturation and swelling of the backfill in the deposition tunnels 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 undesirable change in 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 2-9. Process table for the backfill describing how backfill processes will be handled in different time frames and in the special cases of earthquakes 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 > -2°C. Otherwise discussed	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	Quantitative estimate with an empirical model	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	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. Advective transport of species	Simplified assumptions of mass transport of dissolved species during saturation	Included in geosphere modelling. Cases without the backfill path will be considered	See "Water transport for saturated conditions"
BfT10. Diffusive transport of species	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	Consider varying groundwater composition
BfT11. Sorption (including ion-exchange)	The early stage is not studied specifically, since the conditions in the backfill will be comparable to those for the long-term evolution	Chemistry model	
BfT12. Alteration of impurities	The effect on inorganic reduction of oxygen is modelled	Chemistry model	
BfT13. Aqueous speciation and reactions	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	

	Resaturation/ "thermal" period	Long-term after saturation and "thermal" period	Notes
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 total cation charge is > 4 mM Otherwise modelled	Neglected if total cation charge is > 4 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)	Mass balance considerations	
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 (no failures are expected this period)	COMP23	
BfT22. Transport of radionuclides in gas phase	By-passed (no failures are expected this period)	By-passed	

2.4 Tunnel plug

2.4.1 Initial state of the tunnel plug

The plug is in itself not a barrier but it is a necessary ingredient to help the backfill in the deposition tunnel to maintain its barrier function. The main requirements of the plug are listed below.

- The plug shall seal the deposition tunnel and keep the backfill in place during the operational phase until the deposition and transport tunnels have been backfilled and water saturated, and have regained their hydrostatic water pressure.
- The plug shall resist the hydrostatic water pressure at repository level and the swelling pressure from the backfill and the bentonite seal.
- The plug shall limit water flow from the deposition tunnel past the plug to such an extent that no harmful backfill erosion takes place from the deposition tunnel.
- The plug shall not significantly impair the barrier function of the other barriers.
- The movement of the plug due to pressure shall be within sufficiently small to avoid a drop in backfill density in the vicinity of the plug.

The lifetime of the plug can be divided into three phases with different requirements:

1. Installation phase.
2. Sealing phase.
3. Degradation phase.

There are five different components that constitute the tunnel plugs (Figure 2-3). These are (counted from inside the tunnel and outwards):

1. Drainage material (crushed rock filter) that is used for keeping low water pressure on the concrete plug until it has cured.
2. A bentonite seal built of bentonite blocks.
3. Two walls made of concrete beams with the purpose of supporting the bentonite seal and separating it from the drainage material and the concrete plug.
4. The concrete plug with grouting pipes.
5. Drainage arrangements for pressure control in the drainage material.

The entire plug is thus a composite of different materials with different functions.

1. The drainage material shall keep the pressure from the concrete plug until it has cured. Then it has no function.
2. The bentonite seal shall prevent leakage past the plug after closing the drainage system until full water pressure is reached on both sides.
3. The walls are only required to separate the materials during construction.
4. The concrete plug shall mechanically withstand the water and swelling pressure inside the plug until full water pressure is reached on both sides.
5. The drainage system shall keep the water pressure low in the drainage material.

The concrete part of the plug is constructed from “low-pH” concrete according to the recipes in Table 2-10.

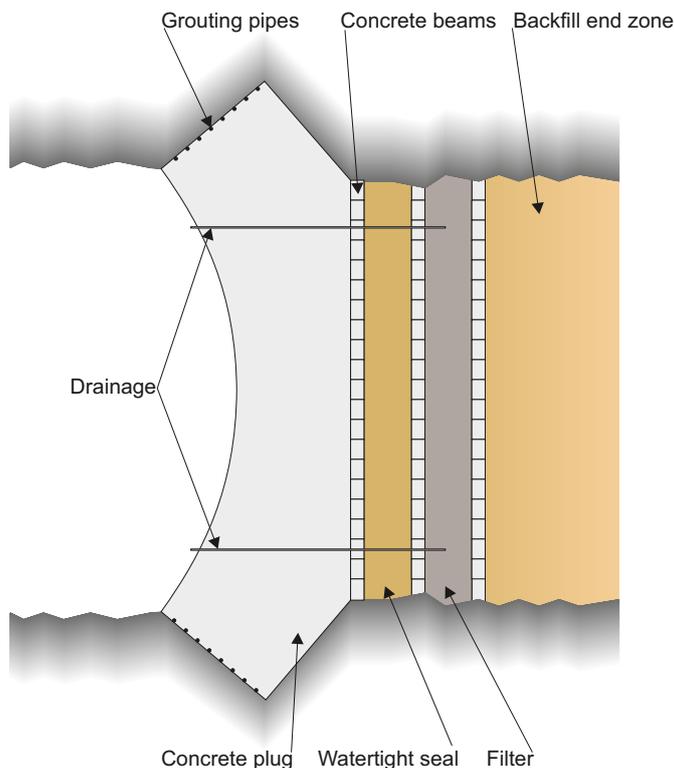


Figure 2-3. Schematic section of the reference design of the plug /SKB 2010e/.

Table 2-10. Reference concrete formulation for the concrete in the plug.

Design parameter	Nominal design [kg/m ³ if not specified]
Binder	
Cement CEM I 42.5 MH/LA/SR	120
Silica fume (densified)	80
Other components	
Water	165
Limestone filler L25	369
Sand 0–8 mm	1,037
Gravel 8–16 mm	558
Glenium 51	6,38
water/cement	1,375 kg/kg
water/binder	0,825 kg/kg
water/powder	0.29 kg/kg

2.4.2 Definition of tunnel plug variables

The tunnel plugs are bounded on the inside by the backfill in the deposition tunnels and on the outside by the backfill in transport tunnels. The plugs are surrounded by the surface of the rock. There will be tunnel plugs separating the transport tunnels from the central area as well.

The tunnel plugs are characterised thermally by their temperature.

No radiation variable is defined for the plugs since the levels of radiation caused by the repository always will remain very low at the positions of the plugs.

Hydraulically, the plugs are characterised by their pore geometry, hydrovariables (pressure and flows), water content, and sometimes by gas content, which are mainly of interest during the period when the plug is being saturated with water.

The plugs are characterised mechanically by their stress state.

The chemical state of the plugs is defined by the composition of the concrete plug, the concrete beams, the bentonite, the drainage and the filter material. The chemical state is also defined by the porewater composition.

The variables are defined in Table 2-11. The initial values of the variables, i.e. the values at the time of deposition, are given in the production line report for the closure /SKB 2010f/.

Table 2-11. Definition of tunnel plug variables.

Variable	Definition
Plug geometry	Geometric dimensions of the plug
Plug pore geometry	Pore geometry as a function of time and space in the components. The porosity (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 the plug
Water content	Water content as a function of time and space in the plug
Gas content	Gas content as a function of time and space in the components
Hydrovariables (pressure and flows)	Flows and pressures of water and gas as a function of time and space in the plug
Stress state	Stress conditions as a function of time and space in the plug
Plug materials – composition and content	Composition of the concrete plug, the concrete beams, the bentonite, the drainage and the filter material in space and time
Plug porewater composition	Composition of the porewater in time and space in the plug
Structural and stray materials	(undefined) The structural materials in the plug are already included in the “Plug materials” variable – stray materials are assumed to be of no concern since no long-term performance is expected from the plug

2.4.3 Summary of handling of tunnel plug processes in SR-Site

Table 2-12 summarises the handling of tunnel plug processes in the safety assessment SR-Site, as suggested in the Process Report. In the table, the process is either “mapped” to a model by which it will be quantified or a brief verbal description of how it will be handled is provided. 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 2-12. Process table for the tunnel plugs describing how tunnel plug processes are handled in different time frames. 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	Notes
Intact canister			
Pg1 Heat transport	Temperature as a function of distance from deposition holes is calculated. However, no specific estimate of the temperature in the plugs is done. The temperature in this component will under all circumstances remain relatively low	Temperature as a function of distance from deposition holes is calculated. However, no specific estimate of the temperature in the plugs is done. The temperature in this component will under all circumstances remain relatively low	
Pg2 Freezing	Neglected, since this requires permafrost conditions	Neglected, since there are no long-term performance requirements on the plugs	
Pg3 Water uptake and transport under unsaturated conditions	THM model	Not relevant by definition	
Pg4 Water transport under saturated conditions	Assumed to be a part of the tunnel with high hydraulic conductivity	Assumed to be a part of the tunnel with high hydraulic conductivity	
Pg5 Gas transport/ dissolution	THM model	Neglected – any effect from the plugs on gas migration would be positive, since they could act as sinks. However, the effect is impossible to quantify	
Pg6 Piping/erosion	The plug is a part in the integrated treatment of piping. However, no assessment of piping in the plug itself is done	Neglected, since piping only occurs during the early part of the repository evolution	
Pg7 Swelling/mass redistribution	THM-model	Neglected, since there are no long-term performance requirements on the plugs	
Pg8 Advective transport of species	Assumed to be a part of the tunnel with high hydraulic conductivity	Assumed to be a part of the tunnel with high hydraulic conductivity	
Pg9 Diffusive transport of species	Neglected since advection will dominate	Neglected since advection will dominate	
Pg10 Sorption	Sorption will occur in the plugs, but is pessimistically neglected	Sorption will occur in the plugs, but is pessimistically neglected	
Pg11 Alteration of concrete	Separate modelling of concrete degradation	Separate modelling of concrete degradation	
Pg12 Aqueous speciation and reactions	Separate modelling of concrete degradation	Separate modelling of concrete degradation	

	Resaturation/ “thermal” period	Long-term after saturation and “thermal” period	Notes
Pg13 Osmosis	Osmotic effects are neglected due to the lack of an osmotic flow in the tunnel	Osmotic effects are neglected due to the lack of an osmotic flow in the tunnel	
Pg14 Montmorillonite transformation	Neglected, since there are no long-term performance requirements on the plugs	Neglected, since there are no long-term performance requirements on the plugs	
Pg15 Montmorillonite colloid release	Neglected, since there are no long-term performance requirements on the plugs	Neglected, since there are no long-term performance requirements on the plugs	
Pg16 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”	Microbial effects in tunnel plugs will be included in the description of the geochemistry in the repository	
Failed canister			
Pg5 Failed canister. Gas transport/dissolution	Assumed to be a part of the tunnel with high hydraulic conductivity (no failures expected in this period)	Assumed to be a part of the tunnel with high hydraulic conductivity	
Pg17 Speciation of radionuclides	Assumptions based on empirical data (no failures are expected this period)	Indirectly accounted for through the selection of parameters for radionuclide transport	
Pg18 Transport of radionuclides in water phase	Assumed to be a part of the tunnel with high hydraulic conductivity (no failures are expected this period)	Assumed to be a part of the tunnel with high hydraulic conductivity	

2.5 Central area

2.5.1 Initial state of the central area

The central area is the assembled part of the sub-surface of the KBS-3 repository facility comprising rock cavities for operation, logistics and maintenance. The rock cavities of the central area shall house transfer of canisters, storage and transshipment of rock masses, buffer, backfill and closure material, storage of equipment etc, garages and workshops, spaces for personnel and visitors and spaces for technical systems.

The central area will be filled with crushed rock. The following is an overview description of the initial state of the central area (Figure 2-4). The initial state for this component is defined as the state at the closure of the repository. A more formal and exhaustive account is given in the production line report for the closure /SKB 2010g/. The repository part that is included in this description is the central area at the repository level where the ramp and shafts for transporting material and personnel start.

The total volume of this area is 125,000 m³. The entire volume is filled with crushed rock from the site. The final density and porosity will be 1,900 kg/m³ and 27% (in the compacted rock fill; 100% in the crown space) respectively. Since crushed rock is a non-swelling material there will be an open gap of about 10 cm in the top of the central area.

2.5.2 Definition of central area variables

Each component in the EBS 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 central area is bounded on one side by the plugs separating the transport tunnels from the central area and on the other side by the plugs separating the backfill in the ramp and shaft from the central area. The central area is surrounded by the surface of the rock.

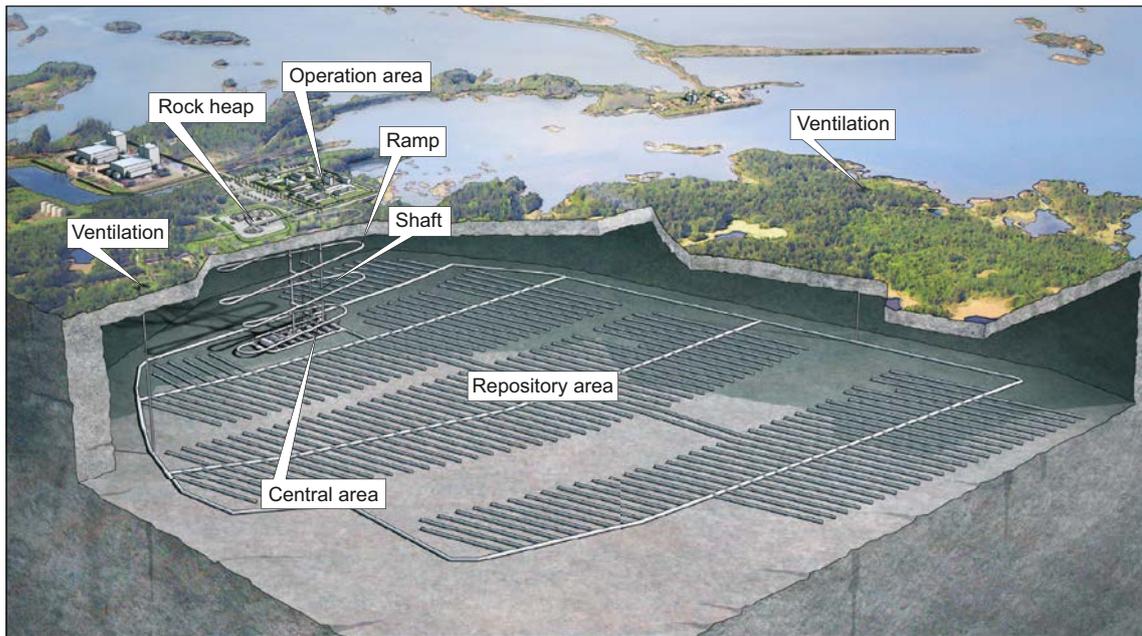


Figure 2-4. The central area of the repository with ramp and shaft /SKB 2010f/.

The central area is delimited by the variable component geometry, which in this case means actual size of the cavern. It is characterised thermally by its temperature.

No radiation variable is defined for these components since the levels of radiation caused by the repository always will remain very low.

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

The central area is characterised mechanically by its stress state.

The chemical state of the central area is defined by the composition of the crushed rock and the structural and stray materials within the component. The chemical state is also defined by the porewater composition.

The variables are defined in Table 2-13. The initial values of the variables, i.e. the values at the time of deposition, are given in the closure production report /SKB 2010f/, the underground openings construction report /SKB 2010g/ and the design report /SKB 2009b/.

Table 2-13. Definition of central area variables.

Variable	Definition
Central area geometry	Geometric dimensions of the component /SKB 2009b/
Central area pore geometry	Pore geometry as a function of time and space in the component. The porosity (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 the component
Water content	Water content as a function of time and space in the component
Gas content	Gas content as a function of time and space in the component
Hydrovariables (pressure and flows)	Flows and pressures of water and gas as a function of time and space in the component
Stress state	Stress conditions as a function of time and space in the component
Central area materials – composition and content	Composition of the crushed rock in time and space in the component /SKB 2008/
Central area porewater composition	Composition of the porewater in time and space in the component
Structural and stray materials	Composition and quantity of construction, reinforcements and stray materials in the component as a function of time and space. /SKB 2010f/

2.5.3 Summary of handling of central area processes in SR-Site

Table 2-14 summarises the handling of central area processes in the safety assessment SR-Site, as suggested in the Process 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 2-14. Process table for the central area describing how the central area processes are handled in different time frames. 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	Notes
Intact canister			
CA1 Heat transport	Temperature as a function of distance from deposition holes is calculated. However, no specific estimate of the temperature in the central area is made. The temperature in this component will under all circumstances remain relatively low	Temperature as a function of distance from deposition holes is calculated. However, no specific estimate of the temperature in the area is done. The temperature in this component will under all circumstances remain relatively low	
CA2 Freezing	Neglected, since this requires permafrost conditions	Neglected, due to small impact	
CA3 Water uptake and transport under unsaturated conditions	THM model	Not relevant by definition	
CA4 Water transport under saturated conditions	Assumed to be a part of the repository with high hydraulic conductivity	Assumed to be a part of the repository with high hydraulic conductivity	
CA5 Gas transport/ dissolution	THM model	Neglected, could potentially be a sink for gas	
CA6 Piping/erosion	Piping in the crushed rock cannot be excluded. However, the central area is always assumed to be a part of the repository with high hydraulic conductivity	Piping in the crushed rock cannot be excluded. However, the central area is always assumed to be a part of the repository with high hydraulic conductivity	
CA7 Swelling/mass redistribution	Most mechanical processes can be neglected since the impact and the requirements on the material are low. However, the interaction between plugs and the central area will be treated in the THM-modelling	Neglected, since there are no long-term performance requirements on the central area	
CA8 Liquefaction	Neglected, since impact is low – if the process occurs at all	Neglected, since impact is low – if the process occurs at all	
CA9 Advective transport of species	Assumed to be a part of the repository with high hydraulic conductivity	Assumed to be a part of the repository with high hydraulic conductivity	
CA10 Diffusive transport of species	Neglected since advection will dominate	Neglected since advection will dominate	
CA11 Sorption	Sorption will occur in the central area, but is pessimistically neglected	Sorption will occur in the central area, but is pessimistically neglected	
CA12 Alteration of the central area backfill	Modelling of the geochemical evolution	Modelling of the geochemical evolution	
CA13 Aqueous speciation and reactions	Separate modelling of concrete degradation	Separate modelling of concrete degradation	

	Resaturation/ "thermal" period	Long-term after saturation and "thermal" period	Notes
CA14 Osmosis	Osmotic effects will be insignificant in the crushed rock material	Osmotic effects will be insignificant in the crushed rock material	
CA15 Alteration of concrete components	Separate modelling of concrete degradation	Separate modelling of concrete degradation	
CA16 Corrosion of steel components	Modelling of the geochemical evolution	Modelling of the geochemical evolution	
CA17 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"	Microbial effects in the central area will be included in the description of the geochemistry in the repository	
Failed canister			
CA18 Speciation of radionuclides	Assumptions based on empirical data (<i>no failures are expected this period</i>)	Indirectly accounted for through the selection of parameters for radionuclide transport	
CA19 Transport of radionuclides in water phase	Assumed to be a part of the repository with high hydraulic conductivity (<i>no failures are expected this period</i>)	Assumed to be a part of the repository with high hydraulic conductivity	

2.6 Top Seal

2.6.1 Initial state of the top seal

The main purpose of the top seal in the upper part of the ramp and shafts is to make unintended intrusion in the repository substantially more difficult. The top seal is defined as the filling in the uppermost 200 m of the ramp and the shafts in the repository. The lower part of the ramp and shaft, extending from 200 m down to the repository is assumed to be filled with backfill material and will have the same properties as the backfill (Section 2.3):

- From 200 to 50 m depth from the ground surface the average hydraulic conductivity of the rock is significantly higher and here is where one can suitably fill the ramp and shafts with crushed rock that has to be effectively compacted to minimise self-compaction under its own weight and overburden.
- The uppermost 50 m of the ramp and shafts should be backfilled with a rock-like material for mechanical protection of the tight, lower parts. It is proposed that residues left over by the quarrying industry forming big heaps at many quarries be trimmed to form a "jig-saw puzzle" with silica concrete poured in the joints. By this means, the ramp and shafts will be sealed with material that resembles host rock with respect to appearance, joints, porosity and resistance to excavation.

The hydraulic properties of these materials have not been measured, but the conductivity can be assumed to be very high, up to ~0.1 m/s.

2.6.2 Definition of top seal variables

Each component in the EBS 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 top seal is bounded on one side by the backfill in the lower part of the ramp and shaft and on the other side by the ground surface. The top seal is surrounded by the surface of the host rock.

The top seal, as it is delimited by the variable geometry, is characterised thermally by its temperature.

No radiation variable is defined for this component since the levels of radiation caused by the repository always will remain very low at the locations of the top seals.

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

The top seal is characterised mechanically by its stress state.

The chemical state of the top seal is defined by the composition of the crushed rock and the structural and stray materials within the component. The chemical state is also defined by the porewater composition.

The variables are defined in Table 2-15. The initial values of the variables, i.e. the values at the time of deposition, are given in the production line report for the closure /SKB 2010f/, the production line for the underground openings /SKB 2010g/ and the design report /SKB 2009b/.

2.6.3 Summary of handling of top seal processes in SR-Site

Table 2-16 summarises the handling of top seal processes in the safety assessment SR-Site, as suggested in the process report. In the table, the process is either “mapped” to a model by which it will be quantified or a brief verbal description of how it will be handled is provided. 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 2-15. Definition of top seal variables.

Variable	Definition
Top seal geometry	Geometric dimensions of the component /SKB 2009b/
Top seal pore geometry	Pore geometry as a function of time and space in the components. The porosity (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 the component
Water content	Water content as a function of time and space in the component
Gas content	Gas content as a function of time and space in the component
Hydrovariables (pressure and flows)	Flows and pressures of water and gas as a function of time and space in the component
Stress state	Stress conditions as a function of time and space in the component
Top seal materials – composition and content	Composition of the crushed rock in time and space in the component /SKB 2008/
Top seal porewater composition	Composition of the porewater in time and space in the component
Structural and stray materials	Composition and quantity of construction, reinforcements and stray materials in the component as a function of time and space

Table 2-16. Process table for the top seal describing how top seal processes are handled in different time frames. 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	Notes
Intact canister			
TS1 Heat transport	Temperature as a function of distance from deposition holes is calculated. However, no specific estimate of the temperature in the top seal is made	Temperature as a function of distance from deposition holes is calculated. However, no specific estimate of the temperature in the top seal is done	
TS2 Freezing	Neglected, since this requires permafrost conditions (probably not entirely true, since the top of the top seal may freeze during winter, see “Long-term”)	The top seal will freeze during permafrost periods. However, the consequences can be neglected due to the high hydraulic conductivity of the material	
TS3 Water uptake and transport under unsaturated conditions	Rough guess of time to reach saturation	Not relevant by definition	

	Resaturation/ "thermal" period	Long-term after saturation and "thermal" period	Notes
TS4 Water transport under saturated conditions	Assumed to be a part of the repository with high hydraulic conductivity	Assumed to be a part of the repository with high hydraulic conductivity	
TS5 Gas transport/ dissolution	Rough guess of time to reach saturation	Neglected – the top seal will have limited effect on gas movement in the repository	
TS6 Piping/erosion	Neglected, since piping cannot occur in the material	Neglected, since piping cannot occur in the material	
TS7 Swelling/mass redistribution	Mechanical processes in the top seal are of no concern for the performance of the repository	Mechanical processes in the top seal are of no concern for the performance of the repository	There will be an interaction between top seal and ramp/ shaft backfill – this is discussed in Section 7.3.1
TS8 Liquefaction	Neglected, cannot occur in this type of material	Neglected, cannot occur in this type of material	
TS9 Advective transport of species	Assumed to be a part of the repository with high hydraulic conductivity	Assumed to be a part of the repository with high hydraulic conductivity	
TS10 Diffusive transport of species	Neglected, since advection will dominate	Neglected, since advection will dominate	
TS11 Sorption	Sorption may occur in the top seal, but is pessimistically neglected	Sorption may occur in the top seal, but is pessimistically neglected	
TS12 Alteration of concrete	Neglected, due to the distance chemical processes in this component will have limited impact on the performance of the rest of the repository. The hydraulic conductivity of this component will under all circumstances be high	Neglected, due to the distance chemical processes in this component will have limited impact on the performance of the rest of the repository. The hydraulic conductivity of this component will under all circumstances be high	
TS13 Aqueous speciation and reactions	Neglected, due to the distance chemical processes in this component will have limited impact on the performance of the rest of the repository	Neglected, due to the distance chemical processes in this component will have limited impact on the performance of the rest of the repository	
TS14 Colloid release	Neglected, will have no effect on the performance	Neglected, will have no effect on the performance	
TS15 Steel corrosion	Neglected, due to the distance chemical processes in this component will have limited impact on the performance of the rest of the repository	Neglected, due to the distance chemical processes in this component will have limited impact on the performance of the rest of the repository	
TS16 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"	No specific treatment of microbial processes in the top seal will be done – is not expected to differ from the rest of the repository	
Failed canister			
TS17 Speciation of radionuclides	Assumptions based on empirical data (<i>no failures are expected this period</i>)	Indirectly accounted for through the selection of parameters for radionuclide transport	
TS18 Transport of radionuclides in water phase	Assumed to be a part of the repository with high hydraulic conductivity (<i>No failures are expected this period</i>)	Assumed to be a part of the repository with high hydraulic conductivity	

2.7 Bottom plate

2.7.1 Initial state of the bottom plate

The bottom plate (Figure 2-5), which consists of a 2 mm thick copper plate on top of a 15 cm thick concrete layer, has only the following two purposes:

- to be a plane, horizontal foundation for the bentonite blocks in the buffer,
- to fasten the temporary bentonite protection (rubber protection sheet and drain tubes, see Figure 2-5) before the pellets are installed. The purpose of the rubber protection sheet and drain tubes is to protect the buffer from water during the installation. They will be removed before the backfill is installed.

There are thus no other demands on the bottom plate after installation other than not to affect the buffer in a negative way. There are, however, several; such effects during the lifetime of the repository that need to be considered.

2.7.2 Definition of bottom plate variables

The bottom plate is bounded on the top by the buffer in the deposition hole and by the bottom and sides of the rock wall.

The bottom plate, as it is delimited by the variable geometry, are characterised thermally by its temperature.

No radiation variable is defined for the bottom plate since the levels of radiation caused by the spent fuel in the canister always will remain low at this location and the radiation will not affect the intended performance of the bottom plate.

Hydraulically, the bottom plate is characterised by its pore geometry, hydrovariables (pressure and flows), water content, and sometimes by gas content, which is of main interest in the phase when the deposition hole is being filled with water.

The bottom plate is characterised mechanically by its stress state.

The chemical state of the bottom plate is defined by the composition of the concrete part and the copper plate. The chemical state is also defined by the porewater composition of the concrete.

The variables are defined in Table 2-17. The initial values of the variables, i.e. the values at the time of deposition, are given in the production line report for the buffer /SKB 2010d/.

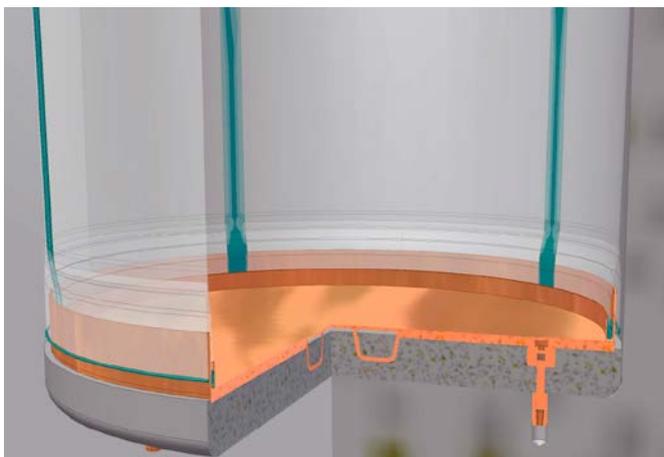


Figure 2-5. The bottom plate (with the temporary rubber protection sheet and drain tubes) /SKB 2010g/.

Table 2-17. Definition of bottom plate variables.

Variable	Definition
Bottom plate geometry	Geometric dimensions of the bottom plate
Bottom plate pore geometry	Pore geometry as a function of time and space in the plate components. The porosity (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 the bottom plate
Water content	Water content as a function of time and space in the bottom plate
Gas content	Gas content as a function of time and space in the bottom plate
Hydrovariables (pressure and flows)	Flows and pressures of water and gas as a function of time and space in the bottom plate
Stress state	Stress conditions as a function of time and space in the bottom plate
Bottom plate materials – composition and content	Composition of the concrete plate and the copper plate
Bottom plate porewater composition	Composition of the porewater in time and space in the bottom plate
Structural and stray materials	(undefined) The structural materials in the bottom plate are already included in the “Bottom plate materials – composition and content” variable – stray materials are assumed to be of no concern since no long-term performance is expected from the bottom plate

2.7.3 Summary of handling of bottom plate processes in SR-Site

Table 2-18 summarises the handling of bottom plate processes in the safety assessment SR-Site, as suggested in the Process Report. In the table, the process is either “mapped” to a model by which it will be quantified or a brief verbal description of how it will be handled is provided. 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 2-18. Process table for the bottom plate describing how bottom plate processes are handled in different time frames. 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	Notes
Intact canister			
BP1 Heat transport	Temperature as a function of distance from deposition holes is calculated. However, no specific estimate of the temperature in the bottom plate is made, since thermal effects on the properties of the bottom plate are disregarded	Temperature as a function of distance from deposition holes is calculated. However, no specific estimate of the temperature in the bottom plate is made since thermal effects on the properties of the bottom plate are disregarded	
BP2 Freezing	Neglected, since this requires permafrost conditions	Of no significance, since no long term performance is expected from the bottom plate	
BP3 Water uptake and transport under unsaturated conditions	The bottom plate is included in the THM modelling of the saturation of the buffer	Not relevant by definition	
BP4 Water transport under saturated conditions	The concrete is included as a component with high hydraulic conductivity	The concrete is included as a component with high hydraulic conductivity	
BP5 Gas transport/ dissolution	No specific assessment of the saturation of the bottom plate will be done	Neglected – any effect from the bottom plate on gas migration would be positive, since it could act as sink for released gas. However, the effect is impossible to quantify	

	Resaturation/ “thermal” period	Long-term after saturation and “thermal” period	Notes
BP6 Piping/erosion	The process does not take place in the bottom plate – but piping in the buffer may be of importance for the interaction with the bottom plate and will be assessed. This is treated in Process BP7	Does not occur	
BP7 Swelling/mass redistribution	Included in THM-modelling	Neglected, of no concern	
BP8 Advective transport of species	Included as a component with high hydraulic conductivity	Included as a component with high hydraulic conductivity	
BP9 Diffusive transport of species	Neglected since advection is likely to dominate – if transport occurs at all	Neglected since advection is likely to dominate – if transport occurs at all	
BP10 Sorption	Sorption may occur in the bottom plate, but is pessimistically neglected	Sorption may occur in the bottom plate, but is pessimistically neglected	
BP11 Alteration of concrete	Separate modelling of concrete degradation	Separate modelling of concrete degradation	
BP12 Aqueous speciation and reactions	Separate modelling of concrete degradation	Separate modelling of concrete degradation	
BP13 Copper corrosion	Neglected, since no long term performance is required from the copper	Neglected, since no long term performance is required from the copper	
BP14 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”	Separate assessment of the reactions that can take place in the bottom plate	
Failed canister			
BP15 Speciation of radionuclides	Assumptions based on empirical data (<i>no failures are expected this period</i>)	Indirectly accounted for through the selection of parameters for radionuclide transport	
BP16 Transport of radionuclides in water phase	Included in COMP23 (<i>No failures are expected this period</i>)	Included in COMP23	

2.8 Borehole seals

2.8.1 Initial state of the borehole seals

A number of more or less vertical investigation or surface-based characterisation boreholes were drilled during the site investigations in order to obtain inter alia data on the properties of the host rock. These boreholes will be sealed no later than at the closure of the final repository. Holes will also be drilled from the repository tunnels during the construction phase, implying that horizontal and upwards directed holes also have to be sealed. Longevity (chemical stability over time) is an essential property of borehole plugs.

Borehole seals will be constructed from compacted bentonite in perforated copper tubes (Figure 2-8). Borehole sections intersected by fracture zones will be filled with concrete (Figure 2-8). In order to minimise the negative impact on contacting clay plugs, the cement content will be very low and low-pH cement will be utilised. Likewise, the amount and type of super-plasticiser, which is required for making the concrete sufficiently fluid, will be kept to a minimum. The cement is not relied on for long periods and it is pessimistically assumed that it will be dissolved and lost, which requires that the physical stability of the remaining sand fill is sufficiently stable to provide the rock and neighbouring clay plugs with adequate support.

The sealing of the upper end of deep boreholes needs to be effective and lasting. Further down in the holes, a “mechanical lock” in the form of a silica concrete plug anchored in a reamed recess will be placed (Figure 2-7). The “lock” will be covered by well compacted till, and trimmed, well-fitting rock cylinders. These covering materials can be allowed to degrade and be lost by glacial erosion, whereas the “locks” need to remain largely intact for protecting the tight seals deeper down. The chemical longevity of the plug materials shall be sufficient to provide adequate sealing of the boreholes for at least 100,000 years. They must have the necessary compressive and shear strengths to withstand the pressure from the tight seals in the holes as well as that arising from potentially high hydraulic gradients.

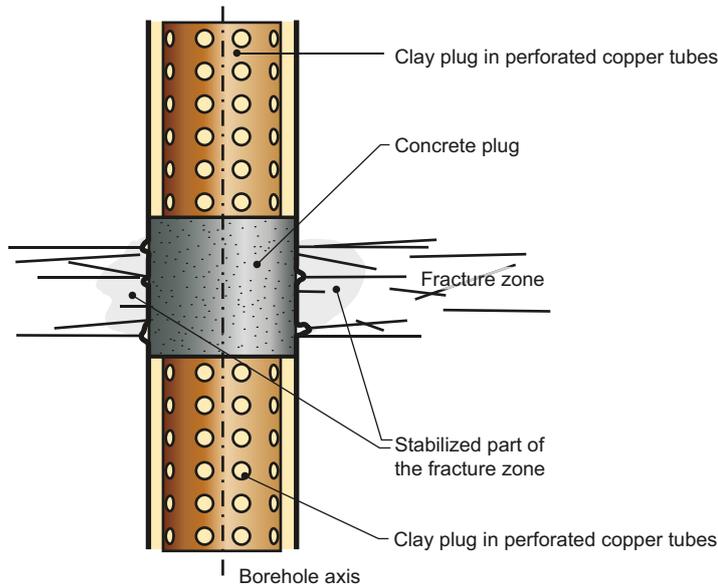


Figure 2-6. Schematic sketch of the construction of concrete plugs in parts where the borehole passes water-conducting fractures /SKB 2010f/.

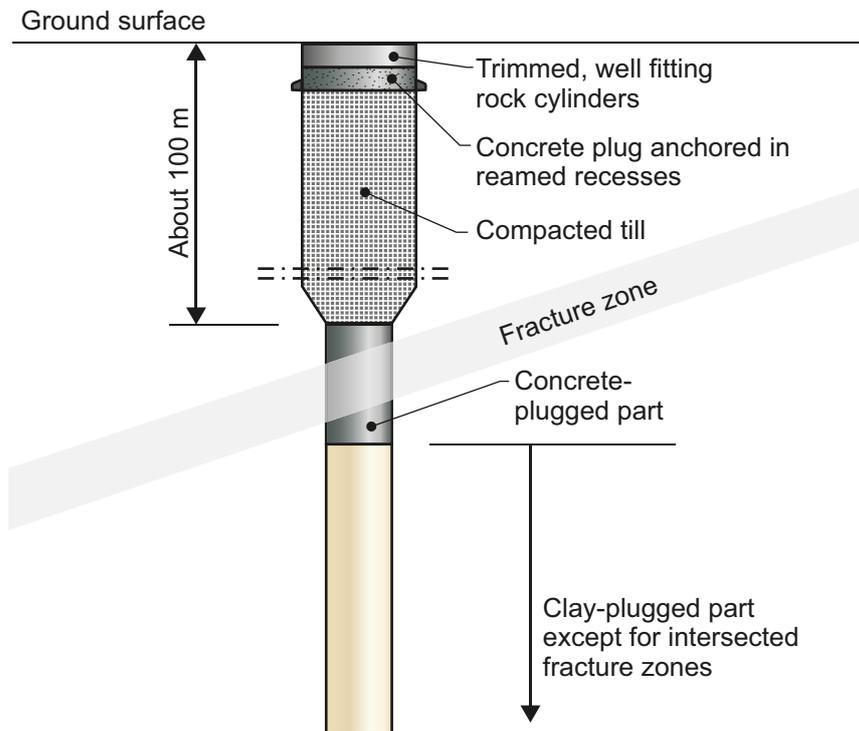


Figure 2-7. The principle for closure of the upper part of a borehole with well compacted till below concrete and fitted rock block /SKB 2010f/.

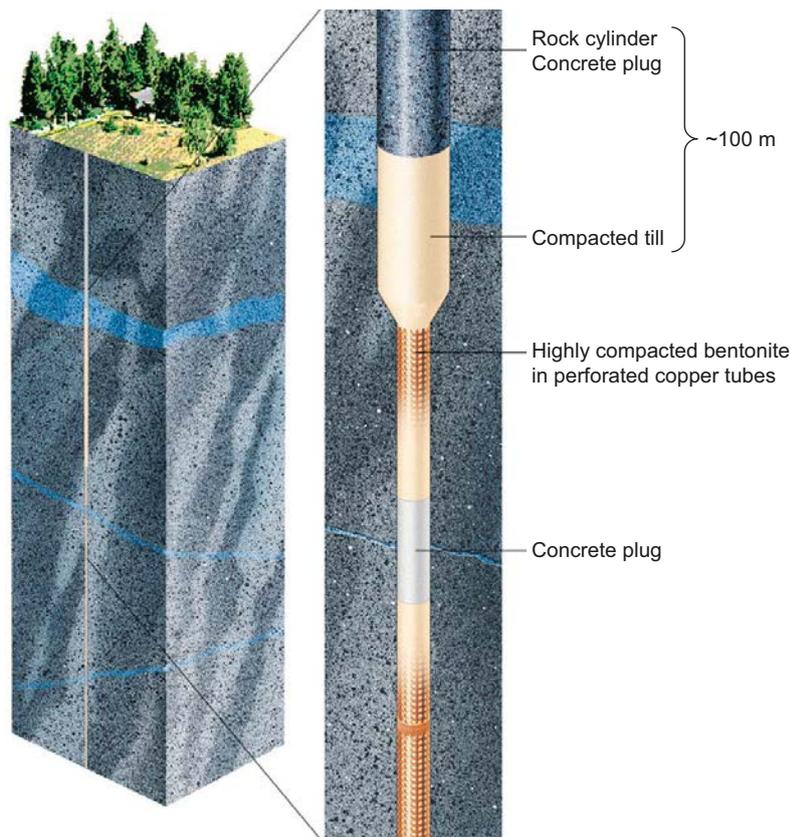


Figure 2-8. Reference concept for sealing investigation boreholes from the surface /SKB 2010f/.

2.8.2 Definition of variables for borehole seals

Each component in the EBS 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 borehole seals are bounded on one side either by the ground surface or by the tunnel backfill. The borehole seals are entirely surrounded by the rock.

The borehole seals, as delimited by the variable geometry, are characterised thermally by their temperature.

No radiation variable is defined for this component since the levels of radiation caused by the repository always will remain very low at the locations of the borehole seals.

Hydraulically, the borehole seals are characterised by their pore geometry, hydrovariables (pressure and flows), water content, and sometimes by gas content, which are mainly of interest in the phase when the bentonite in the seals is being saturated with water.

The borehole seals are characterised mechanically by their stress state.

The chemical state of the borehole seals is defined by the composition of the bentonite, the copper casing and the concrete mixture. The chemical state is also defined by the porewater composition.

The variables are defined in Table 2-19. The initial values of the variables, i.e. the values at the time of deposition, are given in the closure production report /SKB 2010f/.

2.8.3 Summary of handling of borehole seal processes in SR-Site

Table 2-20 summarises the handling of borehole seal processes in the safety assessment SR-Site, as suggested in the Process Report. In the table, the process is either “mapped” to a model by which it will be quantified or a brief verbal description of how it will be handled is provided. 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 2-19. Definition of borehole seal variables.

Variable	Definition
Borehole geometry	Geometric dimensions of the components
Pore geometry	Pore geometry as a function of time and space in the component. The porosity (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 the components
Water content	Water content as a function of time and space in the components
Gas content	Gas content as a function of time and space in the components
Hydrovariables (pressure and flows)	Flows and pressures of water and gas as a function of time and space in the component
Stress state	Stress conditions as a function of time and space in the component
Sealing materials – composition and content	Composition of the bentonite and the concrete in time and space in the component
Porewater composition	Composition of the porewater in time and space in the component
Structural and stray materials	Composition and quantity of construction, reinforcements and stray materials in the components as a function of time and space. This includes the copper tube, the till, rock cylinders and the anchor materials

Table 2-20. Process table for the borehole seals describing how borehole seal processes are handled in different time frames. 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	Notes
Intact canister			
BHS1 Heat transport	Temperature as a function of distance from deposition holes is calculated. However, no specific estimate of the temperature in the borehole seals is made	Temperature as a function of distance from deposition holes is calculated. However, no specific estimate of the temperature in the borehole seals is made	
BHS2 Freezing	A specific assessment of the evolution of the borehole seals during freezing conditions will be done	A specific assessment of the evolution of the borehole seals during permafrost conditions will be done	
BHS3 Water uptake and transport under unsaturated conditions	Assessment of the timescale of borehole seal hydration	Not relevant by definition	
BHS4 Water transport under saturated conditions	Can be neglected as long as the bentonite component remains in place. The case of lost sealing will be assessed in the modelling of the geosphere	Can be neglected as long as the bentonite part remains in place. The case of lost sealing will be assessed in the modelling of the geosphere	
BHS5 Gas transport/ dissolution	No specific assessment of the saturation of the borehole seals will be done. The process is expected to be rather fast since the diameter is small	Neglected – no gas is expected to enter the borehole seals	
BHS6 Piping/erosion	Neglected since the holes are initially water filled and no gradients are expected	Neglected, since piping only occurs during the early part of the repository evolution	
BHS7 Swelling/mass redistribution	Separate modelling of the homogenisation	Assessment of the consequences of a local loss of bentonite	
BHS8 Liquefaction	Neglected, based on same arguments as for the buffer	Neglected, based on same arguments as for the buffer	

	Resaturation/ "thermal" period	Long-term after saturation and "thermal" period	Notes
BHS9 Advective transport of species	Can be neglected as long as the bentonite part remains in place. The case of lost sealing will be assessed in the modelling of the geosphere	Can be neglected as long as the bentonite part remains in place. The case of lost sealing will be assessed in the modelling of the geosphere	
BHS10 Diffusive transport of species	Neglected since diffusive transport in the borehole seals will be very slow	Neglected since diffusive transport in the borehole seals will be very slow	
BHS11 Sorption	Sorption will occur in the borehole seals, but is pessimistically neglected	Sorption will occur in the borehole seals, but is pessimistically neglected	
BHS12 Alteration of concrete	Separate modelling of concrete degradation	Separate modelling of concrete degradation	
BHS13 Aqueous speciation and reactions	Separate modelling of concrete degradation	Separate modelling of concrete degradation	
BHS14 Copper corrosion	Neglected for the tubes, since no long term performance is required from the copper there	Neglected tubes, since no long term performance is required from the copper there	
BHS15 Alteration of impurities in bentonite	Neglected, since no thermal gradients will exist	No specific assessment – the results from the modelling of the buffer will be used as "analogue"	
BHS16 Osmosis	No specific assessment of the saturation of the bore hole seals will be done. The process is expected to be rather fast since the diameter is small. For post saturation, see "long term"	Evaluation of swelling pressure and hydraulic conductivity of the bentonite part of the seals through comparison with empirical data	
BHS17 Montmorillonite transformation	Neglected, process will not occur on short time scale (see long term)	Estimate based on comparison with natural systems. Separate discussion on the interaction between bentonite and concrete	
BHS18 Montmorillonite colloid release	Neglected if total cation charge is > 4 mM Otherwise discussed	Neglected if total cation charge is > 4 mM Otherwise discussed	
BHS19 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"	No specific treatment of microbial process will be done – is not expected to differ from the rest of the repository	
Failed canister			
BHS21 Speciation of radionuclides	Assumptions based on empirical data (<i>no failures are expected this period</i>)	Indirectly accounted for through the selection of parameters for radionuclide transport	
BHS22 Transport of radionuclides in water phase	(No failures are expected this period)	Can be neglected as long as the bentonite part remains in place The case of lost sealing will be assessed in the modelling of the geosphere	

3 Processes in the buffer

3.1 Radiation-related processes

3.1.1 Radiation attenuation/heat generation

Overview/general description

Gamma and neutron radiation from the canister are attenuated in the buffer. The process is described in the Fuel and canister process report /SKB 2010k/. The maximum dose outside the canister has been calculated to be less than 500 mGy/h at time of encapsulation. The dose is dominated by Cs-137, which has a half life of ~ 30 years. The radiation that is not attenuated reaches as far as near-field rock. The main part of the gamma radiation from the spent fuel is shielded by the iron and copper in the canister. Only a minor fraction will reach the buffer.

Radiation is of importance owing to its effect on the chemical processes, principally radiation-induced montmorillonite decomposition and gamma radiolysis of porewater.

Dependencies between process and buffer variables

Table 3-1 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Site.

Table 3-1. Direct dependences between the process “Radiation attenuation/heat generation” and the defined buffer variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence? (How/Why not)	Influence present? (Yes/No) Description	Handling of influence? (How/Why not)
Buffer geometry	Yes. Determines mass/volume available	Included in dose rate calculation	No	
Pore geometry	No		No	
Radiation intensity	Yes. Determines energy deposited	Included in dose rate calculation	Yes. Shielding	Included in dose rate calculation
Temperature	No		Yes. Energy is deposited	Neglected since it is negligible compared to other processes influencing temperature
Water content	Yes. Determines how energy is deposited	Included in dose rate calculation	No	
Gas content	No, but indirectly through water content	See row above	Indirectly through 3.5.13	
Hydrovariables (pressure and flows)	No		No	
Stress state	No		No	
Bentonite composition	Yes. Determines how energy is deposited	Included in dose rate calculation	No	
Montmorillonite composition	Yes. Determines how energy is deposited	Included in dose rate calculation	Yes	Negligible, see 3.5.11
Porewater composition	Yes. Determines how energy is deposited, but the effect is minor	Neglected, Water density does not vary very much	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 3.5.12.

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 outer surface of the canister.

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 3.5.12.

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 over the first 1,000 years. Details of the fuel decay characteristics are provided in Spent Fuel Report /SKB 2010b/.

Handling in the safety assessment SR-Site

Quantification of this process is needed to evaluate the processes 3.5.12 Radiation-induced transformations and 3.5.13 Radiolysis of porewater. The former is shown to be negligible in Section 3.5.12, for the relevant radiation intensities. The latter could affect the canister surface, but also this effect is shown to be insignificant, see further Sections 3.5.13 and the relevant canister process. The radiation field outside a canister has been calculated in /Lundgren 2004/. The calculated dose rate is lower than 500 mGy/h (100–150 mGy/h) at the time of deposition.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

See Fuel and canister process report /SKB 2010k/.

Uncertainties

Uncertainties in mechanistic understanding

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

Model simplification uncertainties in SR-Site

Not relevant.

Input data and data uncertainties in SR-Site

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.

3.2 Thermal processes

3.2.1 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. Initially 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 gaps, 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 pellet-filled gap between buffer and rock will be lower and will not have such a large impact on the canister temperature as the canister/buffer gap. In addition, the pellet-filled gap will start to close soon after deposition while the canister/buffer gap will remain open longer. The efficiency of heat transport through the buffer region is important for the performance of the system, since it affects the maximum buffer temperature for which a design threshold ($< 100^{\circ}\text{C}$) has been established.

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

Shortly 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:

$$\nabla(\lambda\nabla T) = 0 \quad (3-1)$$

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 its density, water saturation and mineral composition. The thermal conductivity of water-saturated MX-80 bentonite that has swelled to its intended density of $2,000 \text{ kg/m}^3$, is about $1.3 \text{ W/(m}\cdot\text{K)}$ according to laboratory experiments.

The thermal conductivity of the pellets-filled gap between the bentonite blocks and the surrounding rock is $0.3\text{--}0.4 \text{ W/(m}\cdot\text{K)}$ /Hökmark et al. 2009/. For the hot air filling the canister-bentonite space, the conductivity is about $0.03 \text{ W/(m}\cdot\text{K)}$, but radiant heat transfer contributes such that the resulting effective conductivity can be set at $0.04 \text{ W/(m}\cdot\text{K)}$ /Hökmark et al. 2009/.

Dependencies between process and buffer variables

Table 3-2 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Site.

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 the 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. The thermal expansion of the buffer material is insignificant.

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. In the unsaturated state, i.e. before swelling and homogenization has started to even out porosity differences, the nominal conductivities of perfectly dry bentonite blocks and perfectly dry bentonite pellets differ significantly. The differences found between the block thermal conductivity (around $1.25 \text{ W/(m}\cdot\text{K)}$) and the pellet slot conductivity (around $0.4 \text{ W/(m}\cdot\text{K)}$) in dry Prototype Repository deposition holes /Hökmark et al. 2009/, is however, also due to differences in initial saturation.

Table 3-2. Direct dependencies between the process “Heat transport” and the defined buffer variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Buffer geometry	Yes	Given as data in the thermal calculation	Yes, but insignificant	Ignored
Pore geometry	Yes	Given as data in the thermal calculation	No, but indirectly via temperature	
Radiation intensity	No		No	
Temperature	Yes. In the unsaturated state, thermally driven vaporization/diffusion/condensation contributes to heat transport	Included in model where appropriate	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, but indirectly via water content		No, but indirectly via water content	
Hydrovariables (pressure and flows)	No		No, but indirectly via temperature and insignificant	Ignored
Stress state	No		No	
Bentonite composition	Yes	Given as data in the thermal calculation	No	
Montmorillonite composition	No		No	
Porewater composition	No		No	
Structural and stray materials	Yes. 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	

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 be ignored for practical purposes. Under unsaturated conditions, vaporization, vapour diffusion and condensation contribute to the heat transport. The contribution is however small and not noticeable other than in the low porosity pellet slot /Kristensson and Hökmark 2010/.

Water content: The thermal conductivity of bentonite depends on the degree of saturation S_r (cf. experimental results shown under “Model studies/experimental studies” below. The conductivity is about 1.3 W/(m·K) for fully saturated bentonite with a KBS-3 buffer density and about 1.0 W/(m·K) if the degree of saturation is 60%. The sensitivity to saturation variations is larger if the saturation drops below 50–60%.

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 away from the canister.

Gas content: 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 insignificant changes to the porewater pressure. During the unsaturated changes there is no or little pressure. During the saturated phase, temperature changes are too slow to impact on the 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 influence 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 montmorillonite is 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 output 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. There is also a dependence on the vertical distribution of the heat generation within the canister, i.e. on the burn-up ratio between the end parts and the mid-parts of the fuel elements. As long as the canister-buffer clearance, or part of that 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 and top. In regions where the clearance is open, part of the flux will be due to heat radiation.

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

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, Ageskog and Jansson 1999, Hökmark et al. 2009/.

These studies have all generated consistent results. The temperature at the buffer/canister transition reaches a peak after about 5–15 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 7.5 m, the tunnel spacing 40 m, the canister output at the time of deposition 1,700 W and the effective rock thermal conductivity 2.6 W/(m·K), the maximum temperature increase at the wall of the deposition hole will be 50°C and about 8°C higher if the canister spacing is 6.0 m. One of the objectives of these studies has to be to find out how the canister spacing influences the maximum rock wall temperature and to establish layout guidelines that ensure that the peak buffer temperature does not exceed 100°C for any canister. 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. The thermal gradients within the buffer are almost zero already after 2,000 years.

/Hökmark and Fälth 2003/ and /Hedin 2004/ used results from different near-field thermal analyses as boundary conditions in numerical and analytical calculations of the heat transfer across the bentonite 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 3-1. The results match well with corresponding results obtained for MX-80 by /Kahr and Müller-Vonmoos 1982/ and with results obtained for similar materials, for instance the bentonite tested in the FEBEX experiment /Huertas et al. 2000/.

The Prototype Repository at Äspö HRL includes six full-scale deposition holes in two tunnel sections separated by a concrete plug /Goudarzi et al. 2003a/. 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 individual holes. The supply of water to the two holes in the outer section is sufficiently low that the inner parts of the bentonite buffer were practically in its initial state of saturation after about 6 months of test operation. The temperature drop across the still open canister/bentonite space in the dry holes was about 19°C 50 days after test start. 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 was almost saturated (i.e. the initial gap was closed) about two years after test start.

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:

$$\lambda_{eff} = \frac{q_c}{\Delta T} \cdot R_c \cdot \ln \frac{R_2}{R_1} \quad (3-2)$$

Here ΔT is the temperature difference between two points at distances R_1 and R_2 , respectively, from the heater axis. R_c is the canister radius. The canister surface heat flux q_c 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 et al. 2009/. Applying the expression to the dry hole in the outer tunnel section described above using data reported by /Goudarzi et al. 2003a/ gives bentonite conductivity values ranging between 1.2 and 1.3 W/(m·K) /Hökmark et al. 2009/.

The TBT (Temperature Buffer Test) experiment in Äspö HRL is run under high thermal gradients and with maximum buffer temperatures well above 130°C /Goudarzi et al. 2008/. The buffer material is MX80 bentonite with the same properties (e.g. density and initial saturation) as the Prototype

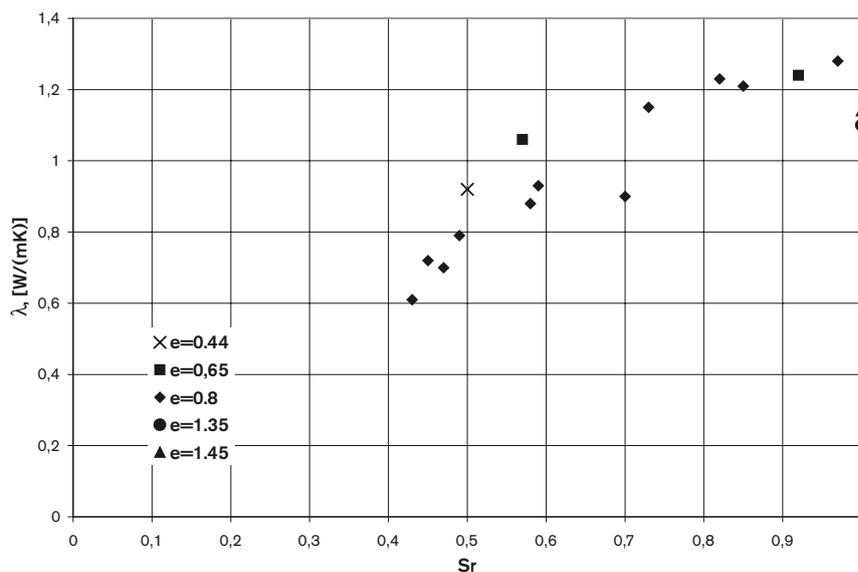


Figure 3-1. Heat conductivity of laboratory-scale bentonite samples as function of saturation for a few values of the void ratio, e /Börgesson et al. 1994/.

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 3-2 above, the thermal conductivity, or rather the change in thermal conductivity, along the scan-line is evaluated and used as an indicator of wetting/drying. The conductivity was found to drop by about 50% in a 0.10–0.15 m wide zone around the heater soon after test start because of drying. Some five years after test start the conductivity has increased and seems to be almost, but not completely, uniformly distributed along the scan-line. This is an effect of water being supplied from the surrounding pressurised sand filter boundary.

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 3.3.1. 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-Site

The integrated thermal evolution of the buffer and rock is modelled with the set of models described in /Hökmark et al. 2009/ and /Hökmark et al. 2010/. Aspects of heat transport relevant to the THM evolution of the buffer are treated in /Åkesson et al. 2010a/.

An important purpose of the modelling is to evaluate the peak buffer 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 transport across these.

The peak buffer temperature will depend not only on the properties of the buffer and the gaps, but also on the repository layout and the rock thermal properties. Therefore the critical temperature calculations were conducted prior to establishing the layout. These calculations are reported in the Site Engineering Report /SKB 2009a/. In SR-Site there are references to the Site Engineering Report and additional evaluations of the results and the relevance of the margins applied in the layout work.

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 /Hökmark et al. 2009/.

Handling of variables influencing the process: The process is coupled to the water saturation process (Section 3.3.1) 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 conservatively neglected. The possibility of moisture being redistributed as a result of vaporisation and vapour diffusion is accounted for by additional margins. The thermal conductivity of the buffer will also be calculated 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 3.3.1.

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, handling of the special cases will be reconsidered.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

The methods used for calculation of the peak buffer temperature are described in detail in the report on strategy for dimensioning of the repository /Hökmark et al. 2009/. The process of selecting buffer parameter values and parameter values for gap properties is described in that same report, which will undergo a documented factual- and quality review. Thermal properties for the buffer used in the calculations of the THM-evolution (Section 3.3.1) are qualified in the THM-data report /Åkesson et al. 2010b/. The principles of rock wall temperature calculations are, in addition to being described in the thermal strategy report /Hökmark et al. 2009/, also described in peer reviewed papers, e.g. /Hökmark and Claesson 2005/. The basis for selection of rock thermal data is found in the thermal site reports /Back et al. 2007, Sundberg et al. 2008/. Both thermal site reports have undergone documented factual- and quality review.

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 in SR-Site

Several modelling simplifications regarding 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 in SR-Site

Critical input data for the modelling of this process will be given in the SR-Site data report /SKB 2010I/. 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. All uncertainties associated with peak buffer temperature calculations are presented in /Hökmark et al. 2009/. Sensitivity calculations will be done to clarify the influence of the various data uncertainties.

3.2.2 Freezing

Overview/general description

The freezing point of a soil is defined as the temperature where ice start to form in the material. The phase transition between ice and liquid state of the soil porewater is affected by pressure and the presence of solutes in the same manner as bulk water. However, the freezing point is generally

depressed in a soil compared to the corresponding bulk solution due to the geometrical constraints of the water in a porous medium. The freezing point of a soil is thus dependent on the stress state, the porewater chemistry, the detailed distribution of the pore volume, the chemical and physical properties of the surfaces of the constituting minerals, and the degree of water saturation.

A further consequence of ice formation taking place in a porous material is that all the porewater will not freeze at one specific temperature. There exists a temperature range below the freezing point where equilibrium exists between ice and water in liquid form. The evidence establishing the existence of a continuous, unfrozen water phase that separates ice from the mineral matrix in porous media such as soils is widely accepted /Anderson 1963, Miller 1963, Nersesova and Tsytovich 1965, Williams 1964/. For a frozen soil, it is therefore relevant to partition the total water content into unfrozen water content and ice content.

$$w = w_u + w_i \quad (3-3)$$

The maximum amount of unfrozen water $w_{u, \max}$ naturally decreases with temperature (keeping all other factors constant). $w_{u, \max}$ depends on various other factors among which particle mineral composition, specific surface area of particles, solute concentrations and pressure are the most significant /Anderson and Tice 1972/. The influence of pressure and solutes is not unique for soil porewater and is known to be such that the freezing point lowers with increasing pressure and solute concentration.

Numerous studies of the relationship between the (maximum) unfrozen water content and temperature, for different types of soils, have been performed; see e.g. /Anderson and Tice 1973, Nersesova and Tsytovich 1965, Andersland and Ladanyi 1994/.

It has been concluded /Anderson and Tice 1972/ that several of the variables describing a specific soil in turn can be related to the specific surface area S , and that a relation between only $w_{u, \max}$, S , and temperature usually gives a satisfactory description (for constant pressure and solute concentration). By fitting a mathematical expression to empirical data for 10 representative soils (isothermal calorimeter measurements), /Anderson and Tice 1972/ achieved the following equation relating maximum unfrozen water content to surface area (m^2/g) and θ , the temperature below freezing ($^{\circ}\text{C}$):

$$\ln w_u = 0.2618 + 0.5519 \ln S - 1.449 S^{-0.264} \ln \theta \quad (3-4)$$

Equation 3-4 can be graphically presented as in Figure 3-2.

Ice will not be present in a soil unless the total water content exceeds $w_{u, \max}$. Hence, Equation 3-4 also gives the freezing point of a soil whose total water amount equals $w_{u, \max}$. Specifically, Equation 3-4 can be used to determine the freezing point of the buffer material.

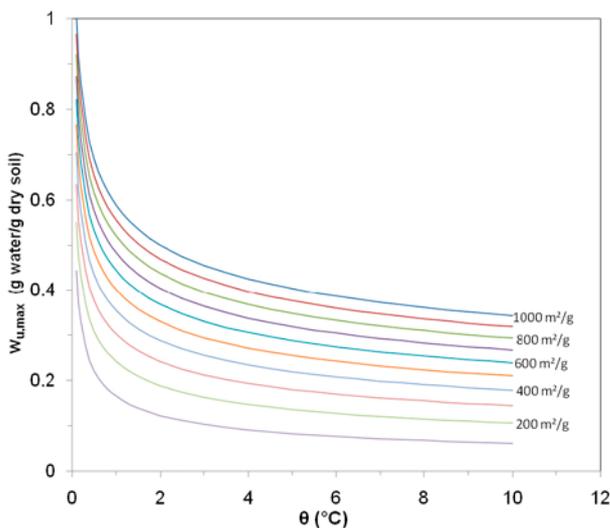


Figure 3-2. Maximum unfrozen water content as function of θ for various values of specific surface areas. θ denotes the number of degrees ($^{\circ}\text{C}$) below the freezing point. (After /Anderson and Tice 1972/).

From Equation 3-4 it is found that a material with a specific surface area of the magnitude 800 m²/g at a temperature of -5°C gives a $w_{u, \max}$ of ca 35%. This value is larger than the total water content of the saturated buffer and from the above it can be concluded that the freezing point of the water-saturated buffer is below -5°C.

The other factors not taken into account in the present estimation (pressure, solutes) of the buffer freezing point will contribute to an even lower value.

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.

Despite the significant freezing point depression in the buffer, the effect of freezing will influence swelling pressure at temperatures above the actual freezing point. Swelling and swelling pressure are phenomena which depend not only on properties of the bentonite itself but also on properties of the external aqueous reservoir. Hence the bentonite swelling pressure will be affected by freezing as soon as the external reservoir freezes.

It is possible to derive the temperature dependence on swelling pressure of a water saturated swelling clay /Birgersson et al. 2008/.

$$P_s(w, T) \approx P_s(w, 0^\circ \text{C}) - \frac{\Delta s(w)}{v_{c.w.}(w)} \cdot T \quad (3-5)$$

where T still denotes temperature below 0°C, $v_{c.w.}(w)$ is the partial molar volume of porewater, $\Delta s(w)$ is the partial molar entropy difference between water in the clay and water in an external ice phase. For values of water content relevant to buffer conditions, $\Delta s(w)$ is of the same order as the molar entropy difference between ice and liquid bulk water (22 J/°C /mol), and a swelling pressure drop with temperature is expected, of the order of 1 MPa/°C. Note, at the temperature given by

$$T_c \approx \frac{v_{c.w.}(w)}{\Delta s(w)} P_s(w, 0^\circ \text{C}) \quad (3-6)$$

swelling pressure is completely lost. This temperature corresponds to the situation when the possible amount of unfrozen water equals the total water content, i.e. expresses the freezing point depression. Assuming a typical buffer swelling pressure above 0°C of 7 MPa and a partial molar volume equal to the value for bulk water (18 cm³/mol) gives $T_c \approx -6^\circ \text{C}$, in good agreement with the Anderson & Tice expression presented in Equation 3-4 and Figure 3-2.

Dependencies between process and buffer variables

Table 3-3 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Site.

Boundary conditions

For the buffer to freeze, the water in the surrounding rock must be present as ice. The ability for (water) mass transport across this boundary is therefore very limited.

Model studies/experimental studies

The swelling pressure response of water-saturated samples of the SR-Site reference material MX-80 at various water contents has been measured down to temperatures of around -10°C /Birgersson et al. 2008, 2010/. A typical result is presented in Figure 3-3. The pressure drop as described by Equation 3-5 was shown to agree quantitatively with measurements. Also the existence of a water content dependent temperature where swelling pressure is completely lost (Equation 3-6) was demonstrated. The processes were shown to be completely reversible during several freezing/thawing cycles. No pressure peaks around 0°C were observed.

Furthermore, the experiments were successfully explained by thermodynamics and the assumption of a homogeneous bentonite with only one type of nm-wide slit like pores. The behaviour was concluded to be completely analogous to freezing point depression in electrolyte solutions.

Table 3-3. Direct dependencies between the process “Freezing” and the defined buffer variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Buffer geometry	Yes. If extended to regions with very low temperatures	Neglected. Large scale freezing is not expected to occur	Yes. Geometry could change through expansion towards the backfill	Neglected. Large scale freezing is not expected to occur
Pore geometry	Yes	See Equation 3-7, which is the main argument why freezing can be neglected	Yes	Neglected, No increase in pressure is expected
Radiation intensity	No		No	
Temperature	Yes	Included in the assessment	No	
Water content	Yes via freezing point and transport capacity	Included in the assessment	Yes, If freezing takes place redistribution of water	Included in the assessment
Gas content	(Yes)	Indirect through water content	No	
Hydrovariables (pressure and flows)	Yes, freezing induces water transport	Included in the assessment	Yes	Included in the assessment
Stress state	Yes, influences the freezing point to a small degree	Neglected, effect is small	Yes. Swelling pressure affected also before ice formation	Calculated/estimated
Bentonite composition	Yes, via The specific surface area	Included in the assessment	No	
Montmorillonite composition	Yes, via the specific surface area and types of counter ions	Included in the assessment	No	
Porewater composition	Yes, influences the freezing point	Neglected, since variations will be small	No	
Structural and stray materials	Yes (potentially)	Neglected, since no stray materials are expected.	No	

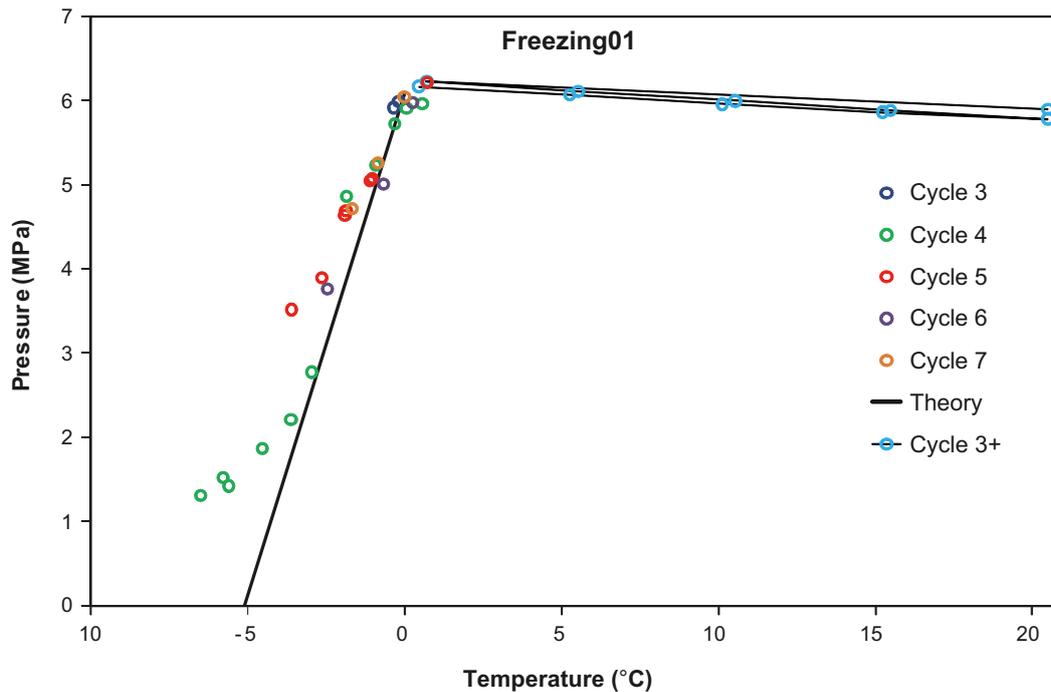


Figure 3-3. Measured swelling pressures below and above 0°C of a sample of MX-80 bentonite which exerts a swelling pressure of approximately 6 MPa at 0°C /Birgersson et al. 2010/. Different colors refers to different freezing/thawing cycles. The theoretical prediction below 0°C (Equation 3-8) is labeled “Theory”.

Natural analogues/observations in nature

No specific studies of natural analogues of frozen clays for the purpose of radioactive waste disposal have been made. However, knowledge can probably be achieved by studying permafrost areas.

Time perspective

The process of freezing is relevant during the entire repository lifetime.

Handling in the safety assessment SR-Site

The freezing process is studied in /Birgersson et al. 2010/. 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. Furthermore, the swelling pressure drop only occurs when the transport paths in the surrounding rock are frozen. Since the buffer is completely recovered at thawing, any deterioration of the sealing properties due to the pressure drop is of no concern. Consequently, the process of freezing of the buffer can be neglected.

Handling of variables influencing the process: The temperature evolution is estimated in /SKB 2010h/.

Uncertainties

Uncertainties in mechanistic understanding

The freezing of soils is a well known process. The description of swelling pressure response due to temperature changes is based on robust, fundamental thermodynamic arguments.

Model simplification uncertainties for the above handling in SR-Site

The reproducibility of the pressure response due to freezing is good. The process can be well described with the equations presented in this section.

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

The bentonite freezing point is strongly dependent on density. If a significant loss of material occurs, e.g. due to chemical erosion, a corresponding change in the freezing behaviour is expected.

The precise value of (minimum) temperature is uncertain. If it stays above 0°C, no phase change at all will occur.

Adequacy of references supporting the suggested handling in the safety assessment SR-site

The supporting references /Birgersson et al. 2008/ and /Birgersson et al. 2010/ are a peer reviewed article and a reviewed report according the SR-Site quality system that are available in the open literature. In addition, these particular studies are aimed directly at dealing with the freezing process in swelling clays.

3.3 Hydraulic processes

3.3.1 Water 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 gradient in negative water pressure or relative humidity 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.

The 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,
 - A2) a temperature gradient
 - 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 porewater pressure, which can be described according to Equation 3-7.

$$\psi = (u_a - u_w) + \pi \quad (3-7)$$

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

The total suction can thus be described from a geotechnical viewpoint as the sum of the matric 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 main driving force for water flow in unsaturated clay is usually considered to be the gradient in porewater pressure, which means that the matric suction and the pore gas pressure are important variables in the modelling of water flow in unsaturated materials. The total suction is a function of the water content of the clay (called retention curve).

The total suction can also be expressed in terms of relative humidity of the clay. Using a thermodynamic approach, total suction is the free energy state of soil water, which can be determined from the partial vapour pressure of soil water /Fredlund and Rahardjo 1993/. Equation 3-8 shows the relation between the partial vapour pressure p and the suction, ψ . The ratio p/p_s corresponds to the relative humidity and Equation 3-8 thus states a strict relation between relative humidity and suction.

$$\psi = - \frac{R \cdot T}{v_{w0} \cdot \omega_v} \ln\left(\frac{p}{p_s}\right) \quad (3-8)$$

where

- ψ = suction (kPa)
- T = absolute temperature (K)
- R = universal gas constant (8.31432 J/(mol K))
- v_{w0} = specific volume of water ($1/\rho_w$ m³/kg)
- ρ_w = density of water (kg/m³)
- ω_v = molecular mass of water vapour (18 kg/kmol)
- p = partial pressure of porewater vapour (kPa)
- p_s = saturation pressure of water vapour over a flat surface of pure water at the same temperature (kPa).

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 complete. 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 the 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 porewater 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 porewater i_c and the temperature T . The porewater 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 and (in the saturated state) the hydraulic head.

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

- A2. The influence of a temperature gradient on the transport of water in the liquid phase is small and mainly indirect via change in water retention properties and water density with temperature except for temperatures below 0°C (see Section 3.2.2 about freezing).

- A3. Transport of water in the 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 the 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.
- A5. Transport of water in the 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 the vapour phase, which is driven by a vapour pressure gradient. The vapour pressure u_v in the fraction of the pores that is air-filled or the relative humidity ($RH = u_v/u_{v0}$ where u_{v0} 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 is re-established. 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 the liquid phase. The relationship between these transport mechanisms has not been fully clarified.
- B2. Transport of water in the 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 some time when the vapour transport is equal to the liquid transport in all parts. A steady-state condition with water ratio differences that reflect the temperature differences in the system will then prevail.
- B3. Transport of water in the 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 the 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, which may be the case 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 the liquid and vapour phases 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 the 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. Parts of the backfill, however, may have such low suction that a pressurised air volume will remain if the air cannot seep out. A large part will disappear 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 room 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.

Dependencies between process and buffer variables

Table 3-4 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Site.

Influence of porewater 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.

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, for buffer densities ($> 1,900 \text{ kg/m}^3$ saturated density) the influence is small also at high salinity.

Influence of hydrovariables: At unsaturated state, the driving force is the matric suction (negative porewater pressure ($u_a - u_w$)). The relation between the total suction (or relative humidity according to Equation 3-8) and the water ratio is called the retention curve. The retention curve under free swelling of MX-80 is shown in Figure 3-4.

The retention curve describes an important relationship for modelling the wetting of buffer materials. It is influenced by a number of factors such as (see /Dueck and Nilsson 2010/):

The wetting path. There is a significant hysteresis effect, which means that wetting yields lower water content than drying at the same RH.

The initial conditions. After mixing with water the measured RH lies between the wetting and drying curve.

The temperature. An increase in temperature yields an increased RH for the same water content.

The confining conditions. If the bentonite is confined and thus not allowed to swell RH will be higher than if it is not confined.

The external stress. An increased external stress increases RH at constant water content.

Influence of temperature: 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. In addition, the temperature influences the retention curve (see above) and the vapour diffusivity.

Influence of water and gas content: The hydraulic conductivity is strongly affected by the degree of saturation. A commonly used relationship between hydraulic conductivity and the degree of water saturation is provided in Equation 3-9.

$$K_p = S_r^\delta K \quad (3-9)$$

where

- K_p = hydraulic conductivity of partly saturated soil (m/s)
- S_r = degree of water saturation
- 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 porewater pressure in an unsaturated buffer is strongly affected by the water content (retention curve). See Figure 3-4.

Table 3-4. Direct dependencies between the process “Water uptake and transport under unsaturated conditions” and the defined buffer variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Buffer geometry	Yes, mainly through distance to wet rock	Given as input data in saturation calculation	Yes. Influencing through the swelling of blocks	See 3.4.1
Pore geometry	Yes, the pore geometry (density) influences the water and vapour transport rate	Included in material data	Yes, through the degree of water saturation that together with the void ratio determines the pore geometry	Degree of saturation and void ratio are calculated
Radiation intensity	No		No	
Temperature	Yes, through water viscosity and through the hydrovariables in a temperature gradient	Included in the models	Yes, through the influence of degree of saturation and void ratio on the thermal properties	Temperature as a function of time and space is calculated for the resaturation phase. See also 3.2.1
Water content	Yes, decisive for the retention curve	Initial water content is given as input data in saturation calculation. The degree of saturation and the void ratio, which determines the water content, are variables in the model	Yes, changes the water content	Degree of saturation and void ratio are calculated
Gas content	Yes, included in the degree of saturation	Initial gas content is given as input data in saturation calculation. The degree of saturation and the void ratio, which determines the gas content, are variables in the model	Yes, changes the gas content	Degree of saturation and void ratio are calculated
Hydrovariables (pressure and flows)	Yes, main variables in the saturation process	Included variables in the saturation calculation	Yes, changes the hydrovariables	Included variables in the saturation calculation
Stress state	Yes, influences the retention curve.	Included variables in the saturation calculation	Yes, changes the swelling pressure	The pressure and suction are calculated
Bentonite composition	Yes, influence through the retention curve and other properties	Included through input data in the saturation calculation	No, unless via mineral conversion	Not relevant for the saturation period
Montmorillonite composition	Yes, influence through the retention curve and other properties	Included through input data in the saturation calculation	No, unless via mineral conversion	Not relevant for saturation period
Porewater composition	Yes, influences the hydraulic properties	Included through input data in the saturation calculation	Yes, through ion transport in a temperature gradient and from absorbed groundwater	See 3.5.6
Structural and stray materials	Insignificant	Excluded, no stray materials are expected in the buffer	No	

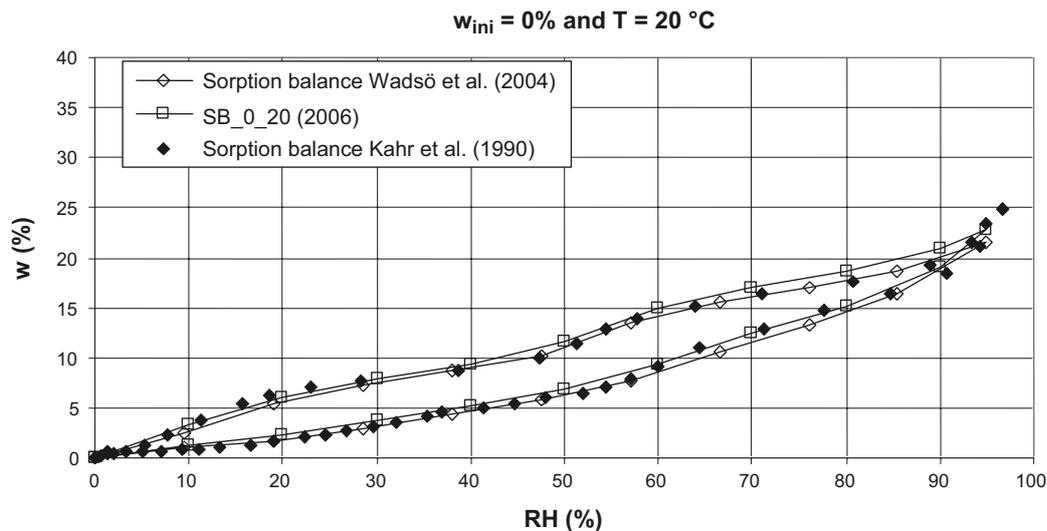


Figure 3-4. Retention curve of MX-80 /Dueck 2004/. The lower curve is absorption and the upper is desorption.

Influence of the stress state

Under volume constraints, the negative porewater pressure is reduced during water uptake and goes to zero (or equals the applied water pressure) at complete water saturation. At the same time, the total pressure from the bentonite towards the confinement increases and reaches the final swelling pressure when the porewater pressure is zero. There is thus interplay between the suction and the external pressure (see also Section 3.4.1).

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: Recently the reference backfill has been changed from a mixture of bentonite and crushed rock compacted in situ to centrally placed clay blocks and pellets in the slot between the blocks and the rock surface. If suction is higher in the buffer blocks than in the backfill blocks, water may be transported from the backfill to the buffer and thus wet the buffer and dry the backfill if the water inflow is very low. 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 material model containing unsaturated water flow has been devised and is being developed. The wetting calculations with this model have been performed using the finite element method with the program Abaqus. Certain general parts of the model are described in the manual /Abaqus manuals/, while other parts are tailor-made for SKB. See e.g. /Börgesson and Hernelind 1999, Börgesson et al. 2005/. 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 several international projects (Äspö TF EBS, DECOVALEX, CATSIUS CLAY and VALUCLAY). These projects include calculation examples and comparisons with measurement results for both laboratory experiments and field tests. See e.g. /Börgesson and Hernelind 1995, Alonso and Alcoverro 2000, Börgesson et al. 2005/.

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). This code is used for modelling e.g. the Äspö HRL large scale tests CRT, Prototype Repository and TBT.

The influence of external pressure and of temperature etc has been investigated in several series of laboratory tests. See e.g. /Dueck 2004, Dueck and Börgesson 2007, Dueck and Nilsson 2010/.

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. 1985/ was performed from 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 the Äspö HRL, several deposition hole tests with heated canister and buffer material are running and two tests have been finished and excavated. These tests are the Canister Retrieval Test (CRT), the Prototype Repository and the Temperature Buffer Test (TBT) /SKB 2005/. 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. CRT was excavated in 2006 about 5 years after installation and a large number of samples taken for measurement of e.g. density and water ratio so that the wetting phase can be studied not only from the results of the sensors measurements but also from the measured state at the end of the test. During 2008, CRT was modelled and the results compared with measurements within the Äspö EBS Task Force. The findings from the Task Force are not reported yet. However, the results are used in the modelling and published within the SR-Site modelling /Åkesson et al. 2010a/.

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 assessment SR-97 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. Additional modelling of the wetting process has been performed and reported by /Börgesson et al. 2006/ and by /Åkesson et al. 2010a/. In the former report special emphasis was given to the influence of the backfill on the wetting of the buffer. However, the backfill was assumed to be compacted in situ. Updating the calculations with the block and pellets backfill is part of the SR-Site modelling programme /Åkesson et al. 2010a/.

The results indicate that wetting takes 5–10 years 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 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 of knowledge with regard to rock properties and buffer/rock interaction and a need for improved material models of the buffer. These matters are a part of the ongoing SKB R&D programme and are included in the Äspö TF EBS (Äspö Task Force on Engineered Barrier Systems).

An extreme case investigated by /Börgesson et al. 2006/ is one where 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.

The other extreme case with no wetting from either rock or backfill 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 initial 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 possibility 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 the vapour flux in the buffer and backfill block pore system and by vapour convection in the pellets pore system.

Additional calculations with sensitivity analyses of e.g. the distance to hydraulic boundaries and some model parameters will be done for SR-Site and reported in the buffer THM modelling report /Åkesson et al. 2010a/. They will also include the new backfill material and further study the drying scenario case 2.

Natural analogues/observations in nature

Wetting of bentonite in nature has not been studied and would probably not contribute to the knowledge necessary for the assessment of water uptake 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 been investigated in a number of calculations /Börgesson et al. 2006/. If wetting is achieved from the backfill (30/70) the time to full saturation of the buffer may be reduced by 50% at normal rock conditions. The calculations is updated for SR-Site.

A very long time until saturation is probably not a problem but the consequences have not been fully investigated (see Model studies).

Handling in the safety assessment SR-Site

A number of calculations of the wetting phase of the buffer with respect to the influence of fracture distribution, distance to hydraulic boundary, backfill conditions and critical parameters of the material models etc are performed for SR-Site and are reported in the buffer THM modelling report /Åkesson et al. 2010a/.

The initial THM evolution covering the saturation phase of the buffer was modelled for a number of hydraulic boundary conditions in SR-Can since the supply of water at the outer buffer boundary strongly influences the wetting rate. The calculations have mainly been made with the old THM-model used for SR-Can /Börgesson and Hernelind 1999, Börgesson et al. 2006/ but updated models, e.g. with Code Bright, are also used in the new calculations. The old calculations have assumed backfill compacted in situ but the revised concept with blocks and pellets is used in the new calculations. 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 is increased knowledge on how much different processes and properties influence the saturation time.

Timescales: The THM modelling encompasses the wetting period for the backfill and buffer. Consequently, the detailed timescale will 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: The process is coupled to a number of other processes in the buffer THM model. The modelling is done for a realistic thermal gradient over the buffer and includes thermal expansion. All influencing variables in Table 3-4 are included in the modelling except effects of varying porewater composition. It is recognised that the salinity of the porewater could influence the final swelling of the buffer. This is, however, included in the near-field evolution model where the effect of salinity on swelling is assessed; see Section 3.5.8 (osmosis).

Handling of variables influenced by the process: As shown in Table 3-4 many of the variables are influenced by the wetting process. These effects are included in the coupled THM-model and are addressed in the THM calculations for SR-Site. 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 walls 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 are calculated.

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.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

The codes used for modelling the initial THM evolution of the buffer are mainly Abaqus and Code Bright. Abaqus is one of the world's leading general finite element codes that undergoes documented quality controls and has been used in numerous applications reported in peer reviewed articles. The material models used for modelling unsaturated buffer materials have been assessed in several international projects (see section Model studies/experimental studies).

Code Bright is a university code that has been designed especially for THM modelling of unsaturated soils. It has recently been made available and the code and the material models are updated regularly and assessed in peer reviewed articles as well as in international projects (e.g. Äspö EBS TF).

The two main reports referred to in the description of the water saturation phase /Börgesson and Hernelind 1999, Börgesson et al. 2006/ are SKB Technical Reports that have not undergone a documented factual- and quality review. However, they are widely referred to by other scientific groups. The revised model of the wetting phase is included in the buffer THM modelling report /Åkesson et al. 2010a/, which will undergo a documented factual- and quality review.

Uncertainties

Knowledge of the hydraulic behaviour of unsaturated buffer material is gained from investigations carried out on MX-80 whereas very few tests have been performed on the other buffer candidate (Deponit CA-N bentonite). At the density considered for the buffer material, their behaviour is expected to be similar but this needs to be confirmed.

Uncertainties in mechanistic understanding

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 are studied in order to gain further confidence in the wetting modelling.

Model simplification uncertainties in SR-Site

The water uptake modelling done so far has assumed that the bentonite blocks and the gaps (filled or unfilled) are homogeneous so that the buffer has uniform density from the start. This simplification is not correct but the error is likely to be smaller than that caused by the uncertainty in the rock properties. Attempts to take these inhomogeneities into account will be made in the CRT modelling and the ongoing development of the codes.

The detailed description of the wetting process is complicated, but it can be modelled with sufficient accuracy for the needs of the safety assessment where it is not necessary for all details of the process to be incorporated. 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 possible chemical alterations of the buffer during the saturation process. Such alterations are, however, not expected to influence the saturation process and hence need not be considered for this process.

Input data and data uncertainties in SR-Site

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

3.3.2 Water transport under saturated conditions

Overview/general description

Water transport in the saturated buffer is a complex interplay between several sub-processes on a microscopic scale. At 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 the saturated buffer is a special case of unsaturated flow. The number of processes to consider is fewer (vapour flux, phase transitions and air phases do not exist). Those processes that are involved are essentially the same as for unsaturated conditions, but can vary widely in importance when compared with unsaturated conditions.

The most important mechanism under saturated conditions is transport of water in the 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 flow-through rate (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 porewater, 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 a density of $2,000 \text{ kg/m}^3$ (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 $D_e = 10^{-12}$ m²/s, which for the buffer thickness $\Delta L = 0.35$ m requires that K exceeds $3 \cdot 10^{-10}$ m/s. This value of K is at least two orders of magnitude higher than the actual conductivity of the buffer. The margin for cations, which have a higher 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 3.5.3.

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

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

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:

$$\sigma_s > 1 \text{ MPa}$$

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.

Dependencies between process and buffer variables

Table 3-5 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Site.

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 3-5 as water content or pore geometry), the ion concentration in the porewater 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 CaN bentonite. The correlation with density is strong. Figure 3-5 and Figure 3-6 show the hydraulic conductivity of MX-80 and Deponit CaN bentonites measured at different densities and with different ion concentrations in the saturating solutions /Karnland et al. 2006/. Blue markers indicate pure water conditions, and these results consequently show the effect of the original 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 end member leads to a hydraulic conductivity similar to those in the original Deponit CaN material, and ion exchange of Deponit CaN clay to the sodium end member leads to hydraulic conductivities similar to those in the original MX-80 clay.

Transformations to other minerals with reduced montmorillonite content generally lead to a higher hydraulic conductivity. 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 not pronounced at buffer densities ($> 1,900$ kg/m³). Results from measurements by /Karnland et al. 2006/ are shown in Figure 3-5 and Figure 3-6.

Influence of stress state

Water is transported into or out from a piece of buffer material when it expands or is compressed. This process is coupled to the mechanical process of swelling and compression, which is treated in Section 3.4.1. The hydraulic part of this process determines the rate of volume change by the time it takes for the water to flow in or out.

Table 3-5. Direct dependencies between the process “Water transport under saturated conditions” and the defined buffer variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Buffer geometry	Yes, mainly by the flow path	Given as input data. The effect of the geometry, meaning how the buffer expands into other volumes (the backfill) is described in Section 3.4.1	Yes, during swelling since water flowing into the voids makes the buffer swell if there is space available for swelling	Included in the mechanical model
Pore geometry	Yes, determines the hydraulic conductivity (see text)	Included in the value of the hydraulic conductivity as a function of the density. The pore geometry can be affected by mineral transformation or a change in porewater composition. The effects are discussed in Sections 3.5.9 and 3.5.8	Yes, during swelling since water flow into the voids makes the buffer swell if there is space available	Included in the mechanical model
Radiation intensity	No		No	
Temperature	Yes, affects water viscosity. The increase of hydraulic conductivity as a function of temperature is about a factor of 3 between 20°C and 90°C	This is neglected in SR-Site because the thermal pulse will be over before any significant radionuclide release may have entered the buffer	Insignificantly. The heat transport due to water transport is very limited	No
Water content	Indirectly through density (pore geometry)		Yes, during swelling since water flow into the voids makes the buffer swell if there is space available	Included in the mechanical model
Gas content	Insignificantly (dissolved gases)	Excluded since it would reduce hydraulic conductivity	No	
Hydrovariables (pressure and flows)	Yes, main variables	Included in the flow model	Yes	Diffusion only for intact buffer. If the hydraulic conductivity once the process is taken into account 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 if advection could be of importance to the system
Stress state	Yes. If the effective stress on the buffer deviates from the swelling pressure the bentonite will change volume and water will flow into or out from it	Included in the mechanical model.	Yes	Included in the mechanical model
Bentonite composition	Yes, determines the hydraulic conductivity (see text)	Included in the model	No	
Montmorillonite composition	Yes, determines the hydraulic conductivity (see text)	Included in the model	No	
Porewater composition	Yes, determines the hydraulic conductivity (see text)	Included in the model	Yes	Replacement of porewater is discussed in 3.5.6
Structural and stray materials	(Insignificant)	Neglected, since no stray materials are expected	No	

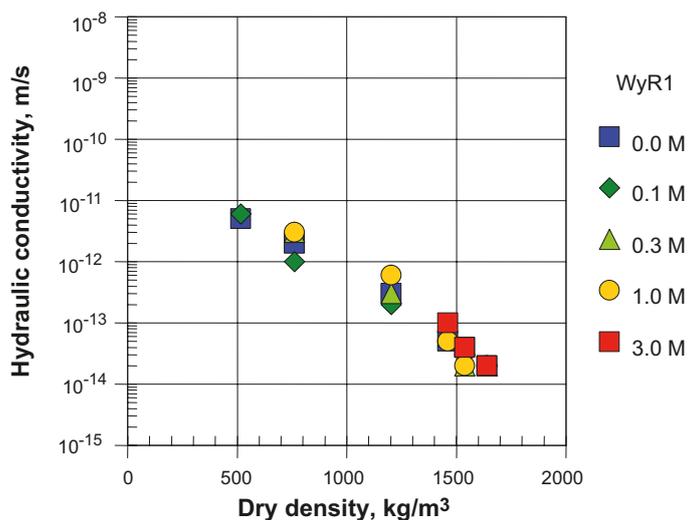


Figure 3-5. Hydraulic conductivity of MX-80(WyR1) bentonite measured at different densities and molar concentration of NaCl in the saturating solution /Karnland et al. 2006/.

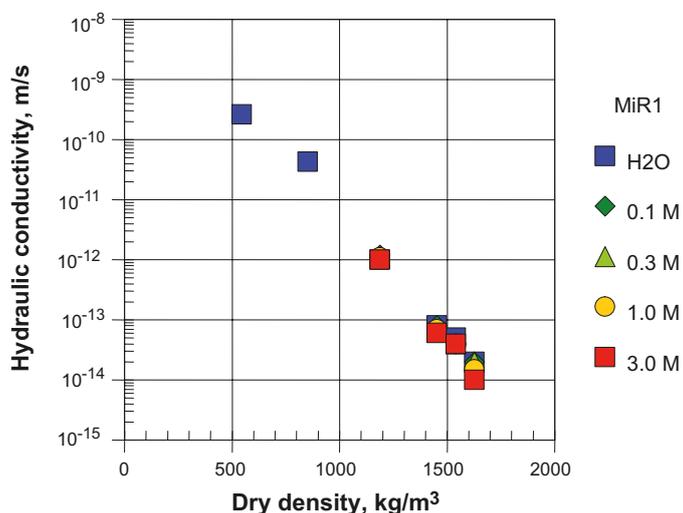


Figure 3-6. Hydraulic conductivity of Deponit CaN(MiR1) bentonite measured at different densities and molar concentration of CaCl₂ in the saturating solution solution /Karnland et al. 2006/.

Boundary conditions

The outer boundary conditions are determined by the hydraulic properties of the backfill on top of the deposition hole and 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 are important.

Model studies/experimental studies

Flow in water-saturated buffer has been studied on the 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 undertaken for several reasons; the main being that the measured values from the laboratory 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 could be considered because they may yield valuable information on long term behaviour.

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. Transport and exchange of ions via advection is thus a slow process compared to ion diffusion (see Sections 3.5.2 and 3.5.3).

The process also affects the rate of swelling into and out from a fracture in contact with the buffer and the rate of homogenisation after full water saturation has been reached.

Handling in the safety assessment SR-Site

The primary handling of this process is 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 is studied and the hydraulic conductivity and the swelling pressure 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 3.4.1.
- The pore geometry can be affected by mineral transformation or a change in porewater composition. The effects are discussed in Sections 3.5.9 and 3.5.8.
- The increase of hydraulic conductivity as function of temperature is about a factor 3 between 20°C and 90°C . This is neglected in SR-Site because the thermal pulse will be over before any significant release of radionuclides to the buffer.
- The hydrovariables are used to calculate the flow in the buffer
- The amount and composition of the swelling component in the bentonite are evaluated according to Section 3.5.9.
- The effect of a change in groundwater/porewater composition are evaluated according to Section 3.5.8.

A combination of several factors will also be discussed.

The hydraulic conductivity is evaluated by application of the empirical relationships described above.

Handling of variables influenced by the process: If the hydraulic conductivity 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 whether advection could be of importance to the system. In this situation, advective transport is included in the calculations of canister corrosion and radionuclide transport.

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

The special cases of failed canister and of earthquakes: These are handled via possible mass redistributions, see Section 3.4.1.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

The main references for results of the hydraulic conductivity measurements on the buffer material and the influence of different factors noted above are /Börjesson et al. 1995/ and /Karlund et al. 2006/. /Börjesson et al. 1995/ is a SKB Technical Report that has not undergone a documented

factual- and quality review. However, it is widely referred to by other scientific groups and can be considered peer reviewed. /Karnland et al. 2006/ has undergone a documented factual- and quality review.

Uncertainties

So far, few tests have been performed on Deponit CA-N bentonite, but the 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 3-6).

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. This is discussed in Section 3.5.9. The effects of very high salinities are also inadequately understood, but this is not relevant for the repository conditions anticipated.

Model simplification uncertainties in SR-Site

The model used is empirical, connecting hydraulic conductivity to temperature, density and ionic strength of the porewater. 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 transport by 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 in SR-Site

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

3.3.3 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 resident in the canister and surrounding buffer, a separate 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 porewater 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 3.3.1. Under these conditions, all gas originally present in the buffer is expected to be dissolved in the buffer's porewater 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 a 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: After saturation, no gas is expected to be present in the buffer unless there is a penetration defect in the canister and water can get into contact with the cast iron insert. The following section only describes the situation with a breached canister.

Diffusion: Hydrogen gas formed by corrosion of the cast iron insert can dissolve in the porewater 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. After the pathway is formed, two different evolutions are possible:

- 1) 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 could be dependent on the swelling pressure. At pressures lower than the shut-in pressure, gas migrates solely by diffusion.
- 2) If the gas production rate is small compared to the permeability of the initial flow path(s), as gas pressure declines, the permeability of the pathways will decline. If gas production is unable to produce sufficient gas to maintain an adequate supply then the aperture of the pathways will decrease (and may well close), potentially resulting in an episodic type response.

Gas entry, breakthrough, peak and steady-state gas pressures in the buffer are dependent on the properties of the buffer and the nature of the boundary conditions. The most important parameters seem to be the swelling pressure, the mechanical properties of the buffer including the stress-strain properties of the clay and host rock and the number, location and geometry of sinks (i.e. host rock fractures) which can accommodate the gas once it has moved through the clay.

Based on the experimental interpretation by /Harrington and Horseman 2003/ for gas tests performed on volumetrically constrained bentonite samples, the peak gas pressure can be expressed as:

$$p_g (\text{peak}) = T + 2\sigma_{eff} + p_w \quad (3-10)$$

based on 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} (see also Section 3.4.1) 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, while a gas phase is present. 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:

$$p_g (\text{post-peak}) = \sigma = \sigma_{eff} + p_w \quad (3-11)$$

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. Under constant volume conditions, the gas pressure cannot fall below the sum of the capillary pressure, p_c , and the externally-applied water pressure (backpressure), p_{we} , or:

$$p_g \text{ (shut-in)} = p_c + p_{we} \quad (3-12)$$

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 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 (performed in low density clays) under unconfined conditions, 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 jeopardising 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 m³), and it is therefore not completely clear what effect the release of large quantities of gas will have on the performance of the repository. However, this aspect of gas migration can be explored through the ongoing Lasgit project /Cuss et al. 2010/ which is a full-scale demonstration test.

Dependencies between process and buffer variables

Table 3-6 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Site.

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 the canister, the backfill and the rock around the deposition hole, the pressure and volume of gas trapped inside the inner interface (the rate/evolution of these components will also influence the gas migration process), and the material properties of the buffer and host rock. The geometric aspects of these boundaries include the nature of the opening in a defective canister, the number, location and geometry of fractures intersecting the deposition hole and the excavation damaged zones around the deposition hole and in the floor of the deposition tunnel.

Once the gas has reached the excavation-disturbed zone (EDZ) in the near-field rock, the pressure required for it to migrate further is much lower than in the buffer. This will result in an expansion of the gas volume and the displacement of porewater around the deposition hole and gallery opening. 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 porewater 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 suction of the bentonite compresses trapped gas (significantly reducing its volume), which is then dissolved in the porewater and this gas is ultimately transported away by diffusion. Gas dissolution essentially follows Henri's law.

Table 3-6. Direct dependencies between the process “Gas transport/dissolution” and the defined buffer variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Buffer geometry	The importance of the buffer volume on gas transport is currently unknown	Assumed to be unimportant	It is important to demonstrate that the gas does NOT influence the buffer geometry	Qualitative assessment
Pore geometry	Is assumed to determine break through pressure – coupled to stress state	See stress state	Fracturing from gas transport	No effect on water transport is assumed
Radiation intensity	No		No	
Temperature	Gas pressure and buffer properties are temperature dependent	Included in the THM modelling of the saturation. For the case of a breached canister this will be neglected since gas transport will take place after the thermal period	No	
Water content	The gas permeability of the bentonite is strongly dependent on the water content	This is considered in the calculation of the saturation process See Section 3.3.1 This will be neglected for a defective canister since in that case gas transport will take place after the saturation phase	The gas may potentially desaturate the clay	Included in the modelling of saturation. This is found to be of limited extent and can be neglected for corrosion gases. A case where contaminated water is pushed out from the canister is assessed within the radionuclide transport calculations
Gas content	See water content	See water content	The gas may potentially desaturate the clay	The de-saturation effect is assumed to be small based on experimental evidence. Diffusive transport of hydrogen is considered
Hydrovariables (pressure and flows)	Gas pressure (gas generation rate) and hydrostatic pressure determine how and when gas can be transported through the buffer	Gas pressure (gas generation rate) is included in the description of the process	The gas pressure is a coupled component in the total near-field pressure	Maximum pressure is estimated
Stress state	The swelling assumed to determine break through pressure in a saturated clay	The swelling pressure is included in the description of the process in the assessment	The gas pressure is a component in the total near-field pressure	Maximum pressure and pressure evolution estimated
Bentonite composition	Indirect influence through stress state		No	
Montmorillonite composition	Indirect influence through stress state		No	
Porewater composition	Indirect influence through stress state		No	
Structural and stray materials	No		No	

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 summarised in /Harrington and Horseman 2003/.

/Harrington and Horseman 2003/ presents the most recent gas migration experiments at laboratory scale within the SKB programme. In the test geometry, the specimen was volumetrically constrained, preventing dilation of the clay in any direction. Figure 3-7 shows the actual test set up. All bentonite specimens were fully hydrated before gas testing by back-pressuring with de-aired and distilled water. This procedure gave initial degrees of saturation that were demonstrably close to 100%.

Figure 3-8 shows a gas injection history from /Harrington and Horseman 2003/ for a laboratory-scale experiment performed on compact bentonite. The test clearly shows the interaction between gas pressure, total stress and porewater pressure during a gas injection history. 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.

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 /Pusch and Forsberg 1983/.

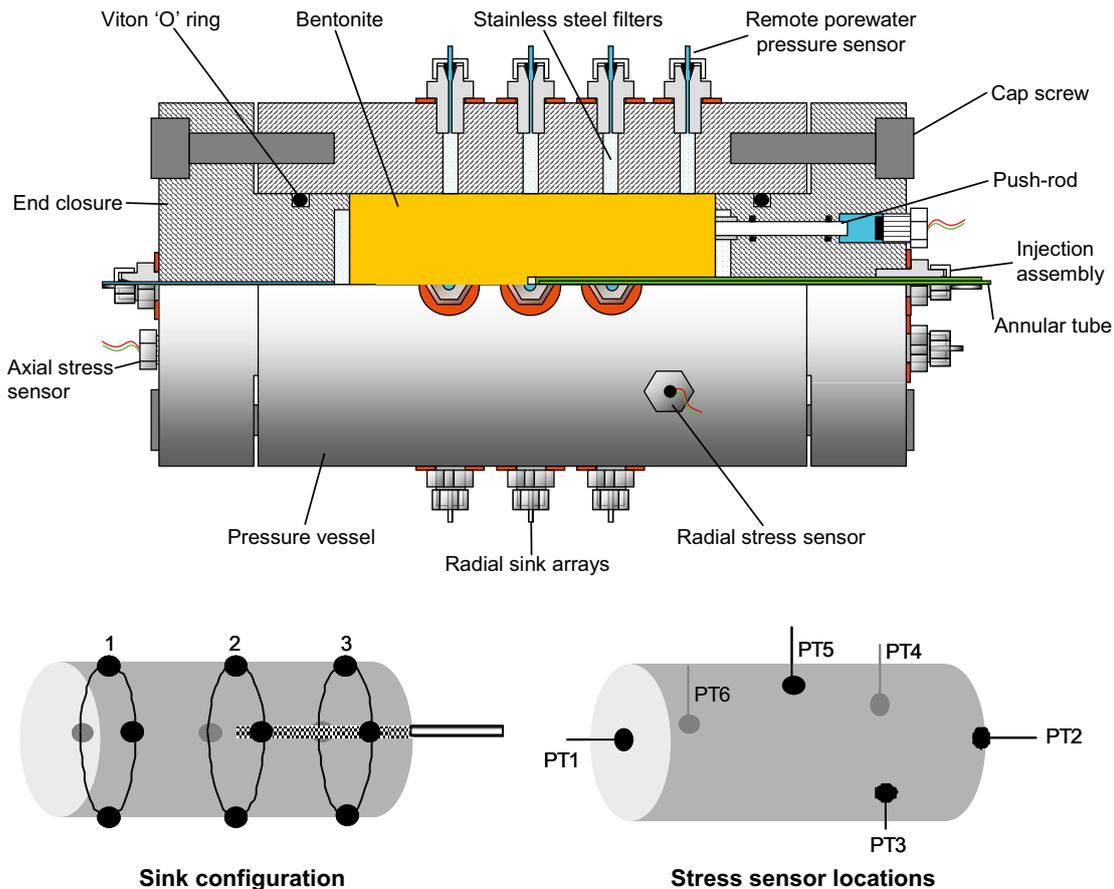


Figure 3-7. Cut-away diagram of the constant volume and radial flow (CVRF) gas migration apparatus /Harrington and Horseman 2003/. [1], [2] and [3] indicates the radial sink arrays. Sensors are as follows: [PT1] – axial total stress on the backpressure end-closure, [PT2] – axial total stress on the injection 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.

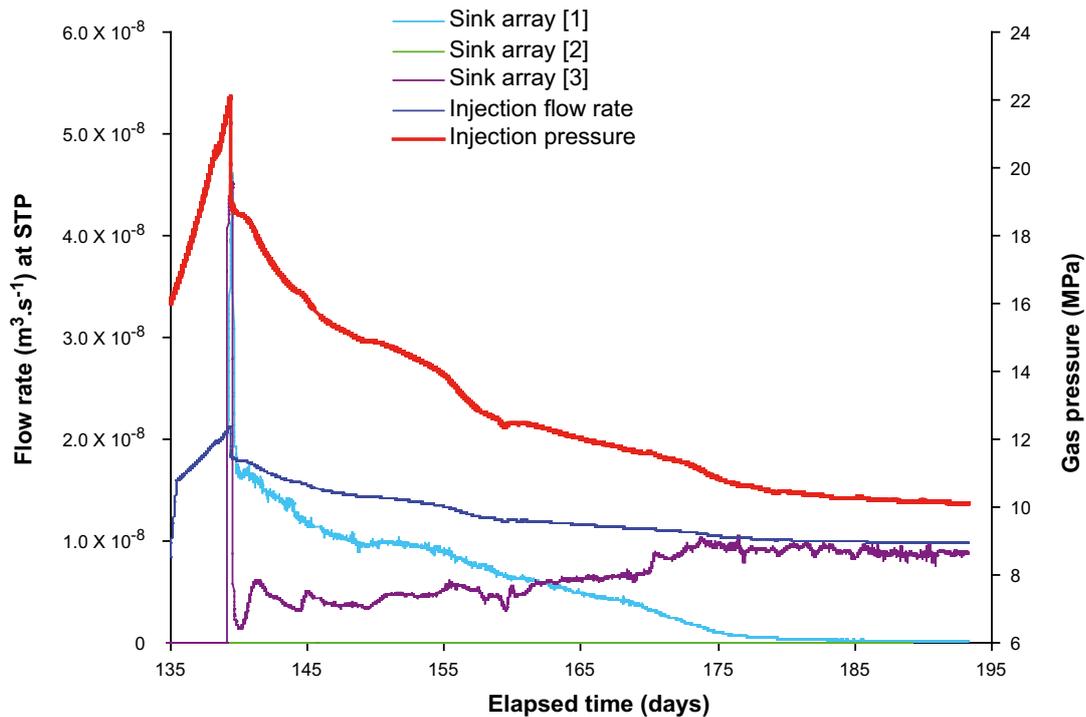


Figure 3-8. Gas injection pressure versus time for the first breakthrough and shut-in stages of test Mx80-10, showing axial and radial total stresses, porewater pressure and flow rate from different sink arrays /Harrington and Horseman 2003/.

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 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 within the Äspö Task Force.

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 conclusions 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 (if any) are displaced, though a case can be made for some degree of dewatering by internal consolidation of the clay at elevated gas pressures.
- 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. The lab results also indicate that gas migration processes are sensitive to the nature of the boundary conditions (i.e. test geometry). The reasons for this remain unclear.

Although there remains uncertainty in the mechanisms of gas migration in bentonite, it is believed that the research into the subject undertaken in a number of laboratories has satisfactorily addressed the key issues with relevance to the effect of gas generation on the safety performance of bentonite buffers in radioactive waste repositories. However, while significant improvements in our understanding of the mechanisms governing gas migration in buffer bentonite have taken place, the paucity of laboratory data available for further model development and calibration (both conceptual and numerical) is a major issue in relation to the quantitative treatment of gas in performance assessment. As an aid to process understanding and model development, additional laboratory tests are required. Uncertainty associated with up-scaling is addressed through the Lasgit international collaborative project.

In the Lasgit, two series of gas injection tests have so far been performed. The first is presented in /Cuss et al. 2010/. In the test a sharp rise in flow rate occurs when the gas pressure is marginally greater (approximately 0.2 MPa) than the local total stress measured on the rock wall, but is around 0.25 MPa lower than the radial stress monitored on the canister surface. The measured axial stress was also marginally higher than the gas pressure (around 0.3 MPa). Gas pressure continues to increase reaching a peak pressure of 5.66 MPa at day 972.3. This is followed by a small spontaneous negative transient leading to a quasi steady state illustrated in detail in Figure 3-9 at a gas pressure of around 5.5 MPa. This behaviour is qualitatively similar to results from laboratory scale tests reported by /Harrington and Horseman 2003/. However, the peak pressure in the field scale test is much lower than in the laboratory tests.

To examine the effect, if any, on the hydraulic properties of the buffer following gas injection, hydraulic tests were performed before and after the gas injection test. Figure 3-10 shows the evolution in flow rate from both hydraulic tests (pre- and post gas injection) plotted against the duration of each test. The tests clearly indicate that little, if any, significant change in permeability has occurred because of the injection of gas. The slight offset in the red line is indicative of a small change in hydraulic storage. Based on the data available, the nascent gas pathways would appear to have no significant effect on the hydraulic performance of the buffer.

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.

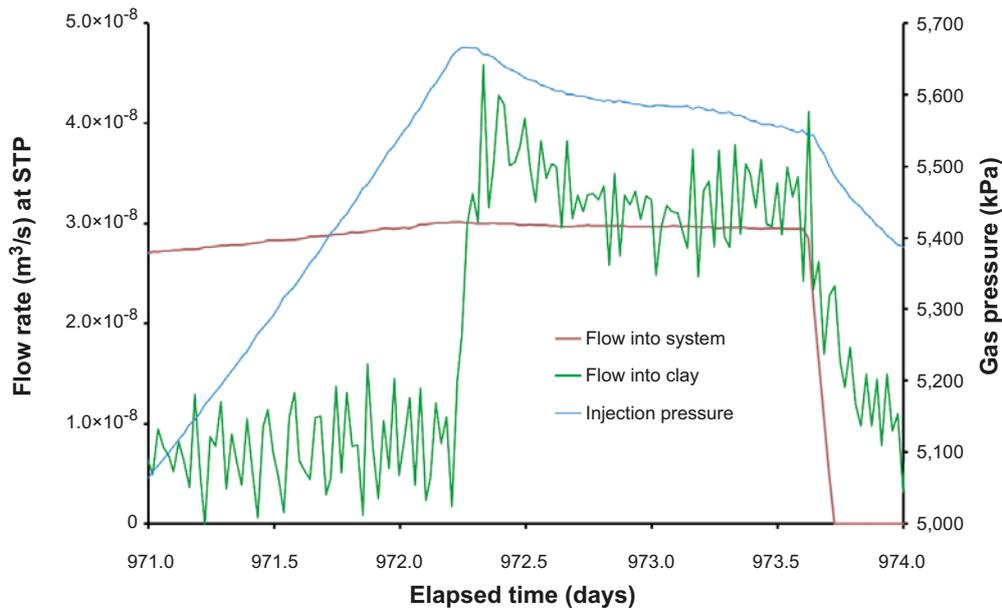


Figure 3-9. Unsmoothed flow rate and pressure responses around peak gas pressure. Gas flow into the clay rapidly increases following the peak which is followed by a small spontaneous negative transient /Cuss et al. 2010/.

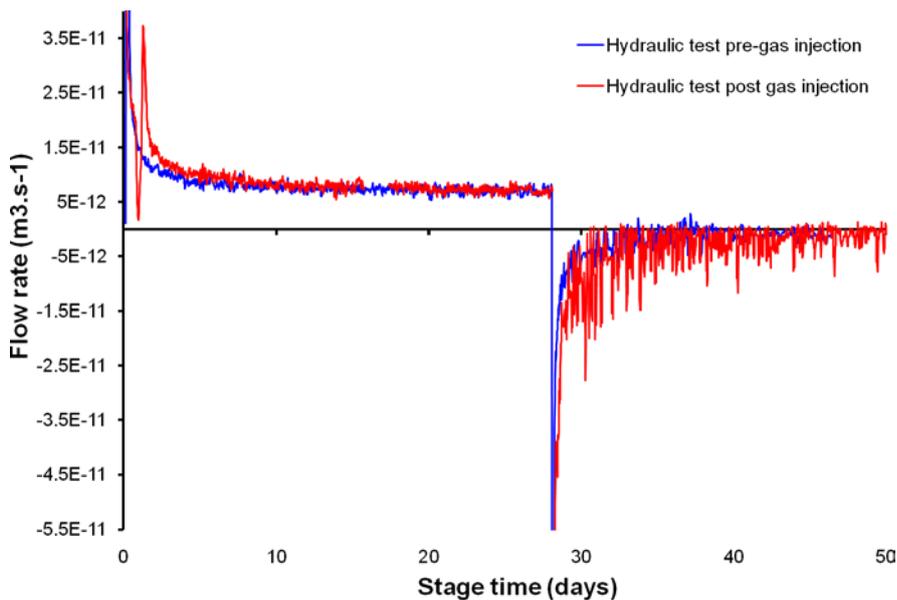


Figure 3-10. Evolution in flow rate for hydraulic tests performed before and after gas injection /Cuss et al. 2010/.

In the context of gas migration in shallow marine sediments, /Judd and Sim 1998/ go so far as to declare “Preliminary modelling suggests that, at shallow subsea depths, gas migration will be initiated by fracture failure rather than capillary migration for all sediment types except coarse sands”. /Clayton and Hay 1992/ extend the debate to argillaceous rocks, suggesting that shaly cap-rocks at current depths of burial less than 500 m are always breached by fracturing, the fracture network providing the main route for leakage of liquid and gaseous hydrocarbons across the cap-rock.

Time perspective

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

Handling in the safety assessment SR-Site

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 built up, this gas volume will have declined by a factor of 50, at an assumed 5 MPa hydrostatic head. The fate of trapped gas is treated in the modelling of the THM-evolution described in Section 3.3.1.

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 not to cause any harm to the other barriers. Gas build-up from corrosion of the iron insert could potentially affect the buffer performance in five 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 damage to the near field rock.
3. The gas could de-water the buffer.
4. A gas phase could push water containing radionuclides through the buffer along gas-generated pathways.
5. Some radionuclides may be transported in a gaseous phase.

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 are 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. The coupling between gas, porewater pressure and stress within the deposition hole and near field are considered.

Model: No quantitative model describing the consequences of gas generation is available, hence the consequences 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 (and porewater 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. Therefore, the corrosion rate primarily determines the rate of pressure increase. This pressure may be transferred to the near-field rock and the backfill. It is assumed that the buffer will open and let the gas through at a certain gas pressure. This maximum pressure is (probably) dependent on the swelling pressure of the buffer. However, while the swelling pressure (at constant volume) is a very important parameter which should be approximately equal to the minimum pressure at which gas remains mobile in the buffer, the maximum gas pressure is strongly associated with the ease at which gas can escape from the deposition hole, i.e. the number, location and geometry of available sinks. If the gas fails to find a sink, the pressure continues to rise. 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-Site Main Report.

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 flammability hazard is not analysed in SR-Site.

Adequacy of references supporting the suggested handling in the safety assessment SR-site

The handling in SR-Site is based on the experimental results by /Harrington and Horseman 2003/. This is a SKB Technical Report which has not undergone a formal peer review. However, the report has been cited by a number of external organisations. The handling of the gas migration in SR-Site is based only on empirical data from the experimental observations by /Harrington and Horseman 2003/. The suggested model in the report, which is described above, is not used in the treatment of the process.

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 features and the volume (stress-strain) behaviour of the clay during gas injection. As mentioned in the Experiments/Models section above, the gas transport observed through bentonite can be interpreted in a number of 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 near field of the repository. Another uncertainty is the closure pressure, the pressure at which the pathways in the bentonite close. A further uncertainty relates to the volume of water displaced during gas flow. Potential de-watering of the clay may affect the engineering performance of the buffer.

These uncertainties are considered in the integrated assessment mentioned above.

Model simplification uncertainties in SR-Site

The evolution of the gas pressure and the gas transport in bentonite in SR-Site is still based entirely on values obtained from experimental results. The complexity of the flow processes and the uncertainties regarding the interpretation of the experiments make predictive modelling difficult at this stage (see above). The paucity of laboratory data available for further model development and calibration (both conceptual and numerical) is a major issue in relation to the quantitative treatment of gas in performance assessment.

Input data and data uncertainties in SR-Site

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, or possibly of the rate with which the gas pressure was increased, but since This aspect of the gas migration process is explored through the Lasgit project and there the maximum pressure was substantially lower /Cuss et al. 2010/ Even with an early failure it would take a very long time to generate a gas pressure. The effect of elevated temperatures on gas pressures can therefore be neglected.

The gas production (corrosion) rate, which determines the timescale of the gas evolution history, is uncertain, as well as the effect of the rate of pressure increase on the process itself.

These data uncertainties are considered in the integrated assessment mentioned above.

3.3.4 Piping/Erosion

Overview/general description

Water inflow into the deposition hole will take place mainly through fractures and will contribute to wetting of the buffer. However, if the inflow is localised to fractures that carry more water than the swelling bentonite can absorb, 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 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 water flow is prevented, must be higher than the sum of the counteracting confining 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 retarded to keep the water pressure at p_{wf} .
3. There is a downstream location available for the flowing water and the removal of eroded materials in order for the pipe to stay open.

Erosion will take place if the drag force on a clay particle from water movement is higher than the sum of the frictional and attractive 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 3.5.11.

The consequence of piping will be a channel and outflow of water to dry or unfilled parts of the repository. Since the clay swells the channel will reduce in size with time but, on the other hand, erosion will counteract and abrade bentonite particles and thus increase the size of the channel. There is thus a competition between swelling clay and eroding clay. If the inflow is low and the increase in water pressure slow the pipe may seal before water pressure equilibrium has been reached.

After complete water saturation and homogenisation of the buffer and backfill and re-establishment of the hydrostatic water pressure the water pressure will be separated from the swelling pressure according to the effective stress theory. The pipes or openings caused by the erosion will thus be sealed and a swelling pressure established if the density and resulting swelling pressure are high enough to overcome internal friction. Later on, there is very little risk of piping since piping requires a strong and fast increase in water pressure gradient locally in the rock at the contact with the buffer or backfill.

The status of knowledge in 2006 is summarised in a report /Börgesson and Sandén 2006/ but additional investigations were performed and reported in 2007 (see below).

Dependencies between process and buffer variables

Table 3-7 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Site.

Boundary conditions

The piping and erosion that are treated here mainly takes place in the pellet-filled gap between the buffer material and the rock.

Model studies/experimental studies

The processes are studied in the following projects

- KBS-3H¹ project.
- Baclo project.
- Buffer installation project.

¹ In the KBS-3H concept, canisters are deposited horizontally in long tunnels, rather than vertically in individual deposition holes.

Table 3-7. Direct dependencies between the process “Piping/erosion” and the defined buffer variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Buffer geometry	Yes, the distance between the bentonite blocks and the rock surface strongly influences the susceptibility 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, through lost buffer material	Amount of lost buffer is calculated
Pore geometry	Yes, by influence of void size distribution in the pellet gap and indirectly through the stress state	Included in the mass balance estimations	No, but indirect through stress state	
Radiation intensity	No		No	
Temperature	No		No	
Water content	Yes, 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 and homogenised	Yes. 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 pellets. Erosion will change the final water content	Amount of lost buffer is calculated
Gas content	Yes, the degree of saturation and the porewater pressure in the backfill influences the risk of piping and the erosion rate	Piping will only occur before the buffer is fully saturated and homogenised	No	
Hydrovariables (pressure and flows)	Yes, basic variables	The hydraulic gradient, the water flow and the duration are included in the estimate of piping and erosion	Yes	The pipes are assumed to seal when the hydraulic gradients are restored. An “after piping” hydraulic conductivity based on the loss of mass is estimated
Stress state	Yes, determines if piping occurs	Included in the consequence estimation	Yes	An “after piping” swelling pressure distribution is estimated
Bentonite composition	Yes, the bentonite and montmorillonite composition affects important variables	Included in the consequence estimation made indirectly through stress state	No	
Montmorillonite composition	Yes, the bentonite and montmorillonite composition affects important variables	Included in the consequence estimation made indirectly through stress state	No	
Porewater composition	Yes, the salinity of the water affects many variables that govern susceptibility to piping and erosion, i.e. the swelling pressure, the swelling rate (through hydraulic conductivity) and the erodability	Included in the consequence estimation since the porewater composition will affect the amount of eroded buffer. However, a conservative upper limit is used in SR-Site	No	
Structural and stray materials	No		No	

KBS-3H

KBS-3H 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. 2005/ and /Sandén et al. 2010/.

The tests show that the bentonite cannot prevent piping and subsequent erosion unless the slot between the bentonite blocks and the rock is very small (a few mm). The tests also show that the process that stops piping is clogging with valve affects rather than derived from swelling pressure. The expected high water pressure in the fractures also tends to deform the bentonite blocks so much that new slots and channels will be formed. The conclusions from the KBS-3H tests and modelling are that it is impossible to prevent piping without building a plug that can withstand the full water pressure. The present design includes water tight end plugs in the deposition tunnels, which limits the effect of erosion to acceptable levels.

Baclo

Tests have been done within the Baclo project in order to investigate the erosion properties of different bentonite materials that may be used both as backfilling blocks and as pellets for filling the slot between the buffer or backfill blocks and the rock /Sandén and Börgesson 2008/.

The results show that the erosion rate depends mainly on the composition of the material, the salt content in the eroding water and the total volume of eroded water, but not so much on the flow rate and the length of the flow path. A reduction in eroding rate with time (or water volume) was also observed. A preliminary model (Equation 3-13) that takes into account the decrease in erosion rate with increasing total volume of eroding water has also been derived /Sandén et al. 2008/.

$$m_s = \beta \times (m_w)^\alpha \quad (3-13)$$

where

m_s = accumulated mass of eroded bentonite (g)

m_w = accumulated mass of eroding water (g)

β = 0.02–2

α = 0.65.

The model is illustrated in Figure 3-11 together with a large number of measurements on different materials under different conditions.

The model may be used for estimating the total amount of eroded buffer material in various situations. The model needs to be checked with additional tests, especially long time tests.

Buffer installation project

The behaviour of the buffer material during the installation phase is investigated in this project. Examples of tests performed include scale tests simulating water inflow into a deposition hole just after filling the slot between the buffer blocks and the rock with pellets. The mechanical effect on the blocks before and after backfilling above the deposition hole and the hydraulic processes occurring when water seeps in from a rock fracture at different inflow rates have been studied. Results to date show that piping and subsequent erosion occurs as expected and that the material eroding out from the hole into the backfill follows Equation 3-13 with low values of the parameter β /Sandén and Börgesson 2010/.

The phenomenon has been observed in two field tests in Äspö HRL (LOT /Karnland et al. 2000/ and in the full scale test Lasgit /Cuss et al. 2010/). 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.

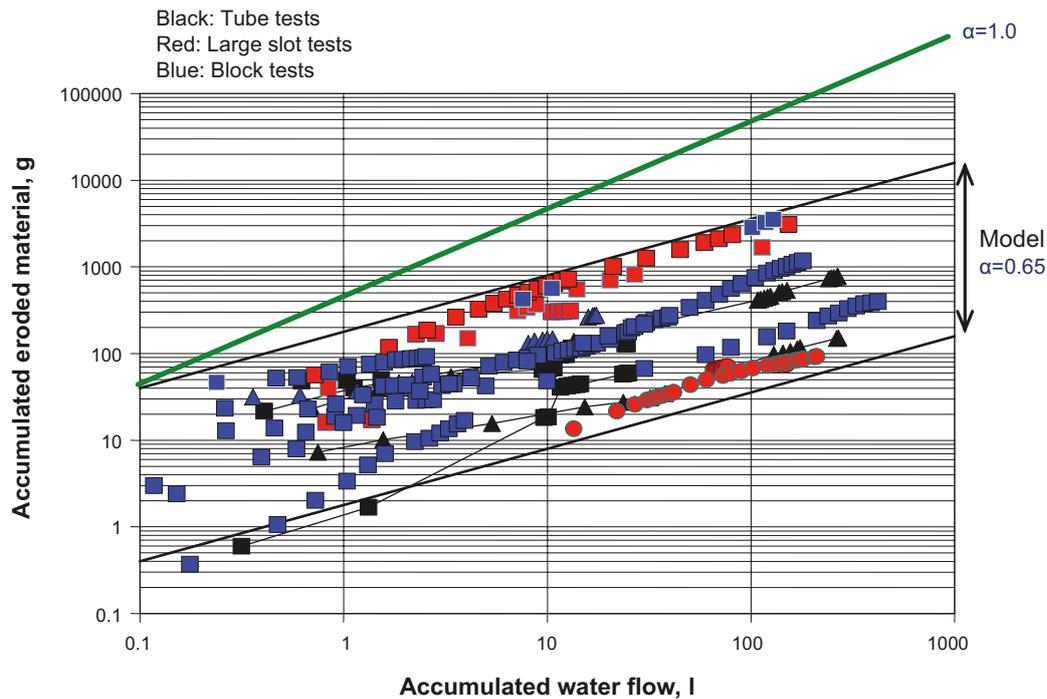


Figure 3-11. Illustration of Equation 3-13 together with results from different erosion measurements on various bentonite materials. α corresponds to the inclination of the straight line in the logarithmic diagram. /Sandén et al. 2008/.

Natural analogues/observations in nature

Piping and erosion may occur in natural deposits but has so far not been studied. The very special circumstances with the high water pressure at repository depth make such observations doubtful.

Time perspective

The piping and erosion (excluding colloid erosion) takes place only 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 porewater pressure in the buffer will always be higher than the external 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-Site

The consequences if piping and subsequent erosion may be severe since the process cannot be stopped by the swelling bentonite in the deposition hole until either a large part of the buffer is saturated and piping is stopped by the swelling pressure or until the voids in the buffer and backfill have been filled with water and the water pressure gradient is taken up by the plug in the deposition tunnel (see the general description). The consequences of erosion are estimated for different inflow scenarios. If the consequences are unacceptable, the deposition hole will be abandoned.

Model: The maximum consequences of this process are estimated by model calculations. This is based on experience from the studies reported and the model according to Equation 3-13.

Time periods: The piping/erosion process is only relevant during the installation and saturation period 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 rate of increase in water pressure are the key variables for this process. Erosion is also affected by the geometry of the initial gaps in the system. The effect of the salinity of the groundwater is also included in the description. All of these variables are included in the preliminary model.

Handling of variables influenced by the process: The consequence of extensive piping together with erosion would be a loss of buffer density, which is calculated for different cases.

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

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

Equation 3-13 is used to estimate the effect of erosion of bentonite from a deposition hole. The basic reference for this model is /Sandén et al. 2008/ although this report refers to backfill material. Tests more relevant for the conditions in a deposition hole are ongoing and will be reported and evaluated in the same way. /Sandén and Börgesson 2010/. This report and the modelling report /Åkesson et al. 2010a/ will undergo a documented factual- and quality review.

Uncertainties

Uncertainties in mechanistic understanding

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. Furthermore, the time required for the buffer to seal such an inflow from a fracture is not known. Until a limiting inflow that can be handled by the buffer without erosion of bentonite out from the deposition hole is found; the consequences of erosion must be considered.

Knowledge of when piping and erosion might occur and the consequences are not fully understood at present. Further tests are ongoing and planned.

Model simplification uncertainties for the above handling in SR-Site

The model is based entirely on empirical data.

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

The constants used in the model are derived from a set of measured data. The spread of the measurements is large.

The boundary condition for this process is the inflow to the deposition hole, which is expected to vary widely.

3.4 Mechanical processes

3.4.1 Swelling/mass redistribution

The swelling process has been combined 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 reaches its peak at full water saturation.

In a deposition hole, the buffer is initially inhomogeneous due to the gaps between the buffer blocks and the rock and canister surfaces. When water from the rock fills the outer pellet-filled slot and enters the bentonite blocks there will be swelling of the blocks and compression of the pellet filling in the outer slot. At first the swelling will be pronounced because of the overall low bulk density of the pellet-filled slot. The resistance to compression is 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, saturation is achieved and the compression of the outer part and the expansion of the inner part will come to some kind of equilibrium. This will not 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.

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 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 3.5.11). Besides mechanical 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 porewater.

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 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 porewater. 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 porewater in the water menisci on the surface of the specimen. The negative pore pressure is equal to the 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 porewater 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 porewater pressure is kept positive, the entire swelling pressure becomes an external pressure. At water saturation, the swelling pressure and the porewater pressure are independent quantities and give a total pressure that is the sum of the pressures (effective stress theory) according to Equation 3-14.

$$\sigma = \sigma' + Au \quad (3-14)$$

where

σ = total stress

σ' = effective stress = swelling pressure

u = porewater pressure

A = 1.0 for normal soils.

Dependencies between process and buffer variables

Table 3-8 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Site.

The data and discussion of 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.

Table 3-8. Direct dependencies between the process “Swelling/mass redistribution” and the defined buffer variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Buffer geometry	Yes. 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 included in the model
Pore geometry	Yes. Through void ratio and indirectly through stress state	Void ratio is included in the model	Yes. Through void ratio and indirectly through stress state	Void ratio is included in the model
Radiation intensity	No		No	
Temperature	Yes, by thermal expansion and indirectly via the hydro-variables	Excluded from assessment (see below)	(Insignificantly)	
Water content	Yes, decisive variable	Included in THM modelling of unsaturated buffer	Yes	Included in THM modelling of unsaturated buffer
Gas content	Yes, degree of saturation is a model variable	Included in THM modelling of unsaturated buffer	Yes, degree of saturation is a model variable	Included in THM modelling of unsaturated buffer
Hydrovariables (pressure and flows)	Yes, model variables	Included in THM modelling of unsaturated buffer	Yes, model variables	Included in THM modelling of unsaturated buffer
Stress state	Yes, model variable	Included in THM modelling of unsaturated buffer and included in calculation of the mechanical interaction with the canister as well as backfill	Yes, model variable	Included in THM modelling of unsaturated buffers and included in calculation of the mechanical interaction with backfill
Bentonite composition	Yes, influences the suction potential and the swelling pressure	The initial composition of the buffer is the starting point of the evaluation	No	
Montmorillonite composition	Yes, influences the suction potential and the swelling pressure	The initial composition of the buffer is the starting point of the evaluation	No	
Porewater composition	Yes, influences the suction potential and the swelling pressure	Included in the model via the suction potential and the swelling pressure etc	No	
Structural and stray materials	Unclear	Not considered with the SR-Site assessment, since no stray materials are expected in the buffer	No	

Measured swelling pressure at constant volume after water saturation is shown in Figure 3-12 and Figure 3-13 for both MX-80 and Deponit CA-N bentonites /Karnland et al. 2006/. The influence of density and ion concentration in the saturating water is measured and included in the figures. Similar investigations have been undertaken by /Börgesson et al. 1995/.

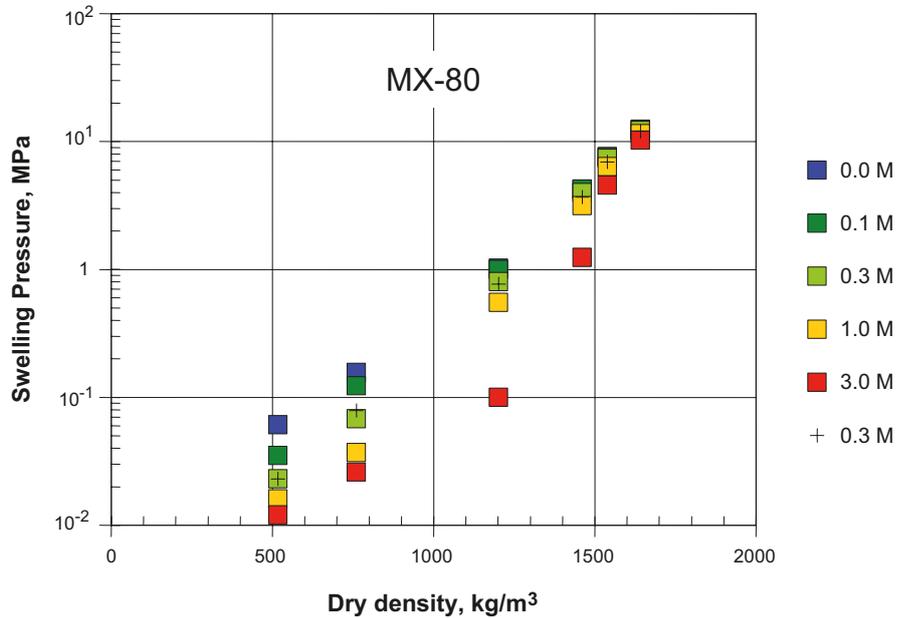


Figure 3-12. Swelling pressure of MX-80 bentonite measured at different densities and molar concentration of NaCl in the saturating solution. All tests have been performed with increasing salt concentration except for the tests denoted +, which have been performed after reduction in salt concentration from 3 molar /Karnland et al. 2006/.

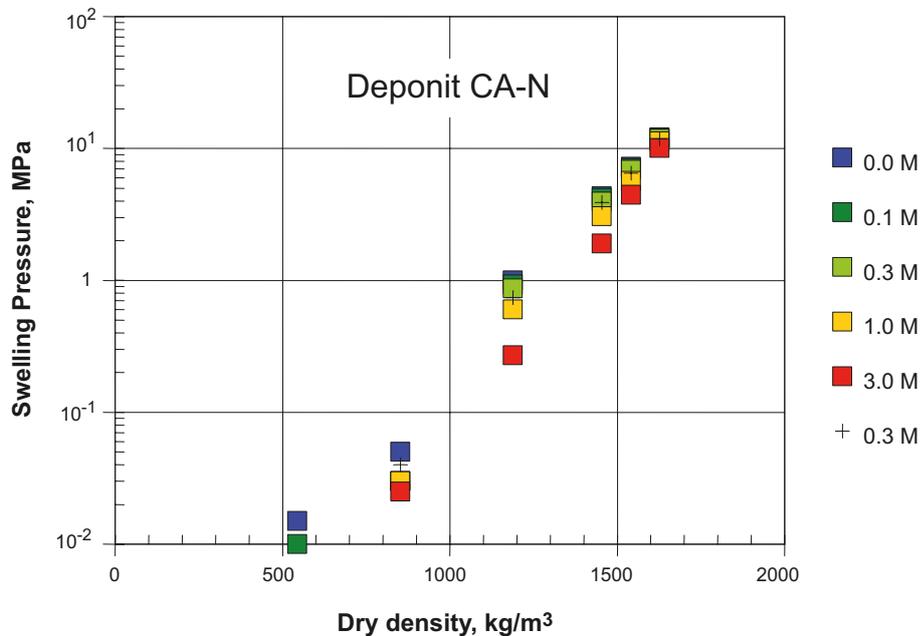


Figure 3-13. Swelling pressure of Deponit CA-N bentonite measured at different densities and molar concentration of CaCl₂ in the saturating solution. All tests have been performed with increasing salt concentration except for the tests denoted +, which have been performed after reduction in salt concentration from 3 molar /Karnland et al. 2006/.

Influence of density: The density at water saturation is decisive for the water ratio, which determines the swelling pressure. Figure 3-12 and Figure 3-13 illustrate the difference in swelling pressure at different densities and ion concentrations in the saturating water /Karnland et al. 2006/.

Influence of montmorillonite content and species of adsorbed cation: According to Figure 3-12 and Figure 3-13 the swelling pressure is relatively independent if the adsorbed ion is sodium or calcium, if the density at saturation exceeds approximately $1,800 \text{ kg/m}^3$ and the montmorillonite contents 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 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 porewater: Increased ion concentration in the groundwater generally leads to a reduced swelling and thereby to effects on the pore geometry that are similar to those of ion exchange to divalent ions. The increase in 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 ($< 1,800 \text{ kg/m}^3$) (see Section 3.5.8).

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 may differ between the unsaturated and the saturated state, since the swelling in unsaturated state 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.

The mechanical properties of unsaturated bentonites are complicated. Different models are used in Abaqus and Code Bright. A new model that takes into account the thermo-mechanical interplay between suction and swelling pressure has been suggested /Dueck and Börgesson 2007/.

If volume is constrained 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 than measured under ideally confined conditions 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 change volume, which 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 also rather small /Villar 2002/ and /Dueck and Nilsson 2010/ and mainly concerns the retention curve. At temperatures below zero the effect is very strong; see Section 3.2.2 on freezing.

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 water 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 resistance other 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 porewater (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. There is also an additional influence of temperature on the retention curve with similar consequences.

The consequences can be more serious in water-saturated buffer, since there are no gas-filled pores to accommodate 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, its volume expansion is large and its compressibility low. Theoretically, the resultant pressure increase against the surroundings can amount to several tens of MPa for 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 parallel with the temperature increase. This process of excess pore pressure dissipation is relatively fast and will greatly reduce the pore pressure increase if the temperature increase is slow and a drainage path is available.

Influence of high water pressure

The effective stress (Equation 3-14) has been shown to be valid for most soils at relatively low stresses and water pressure. However, for bentonites such as MX-80, high water pressure seems to invalidate this equation in the sense that $A \neq 1$. However, the deviation is not strong since the value of A is between 0.9 and 1.0 depending on density and water pressure /Harrington and Birchall 2007/.

Boundary conditions

The boundary conditions of interest mainly concern the interaction between the buffer's interfaces with the near field rock, the canister and the deposition tunnel backfill.

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

Owing to friction against the rock and friction in the buffer, homogenisation 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 and ultimately reaches the average density at some distance from the interface.

Figure 3-14 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 heave 5–10 mm due to the uneven wetting of the buffer but settle at completion of the wetting and ultimately reach their initial position. The results also show that after full saturation and complete consolidation the density and swelling pressure are reduced above the canister but not along the sides of the canister.

Upwards swelling for different backfill types and backfill densities have been investigated with analytical calculations /Johannesson and Nilsson 2006/. They were made in order to find the required density of different backfill materials in order not to lose too much in buffer density on top of the canister ($> 1,950 \text{ kg/m}^3$). Additional modelling is ongoing and will be presented as a part of SR-Site /Åkesson et al. 2010a/.

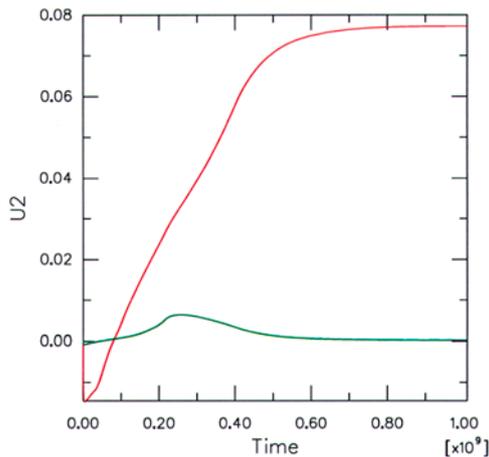


Figure 3-14. Heave (m) of the buffer/backfill interface (red) and the canister (green) as a function of time (s) elapsed from deposition. Example from a FE-calculation /Börgesson and Hernelind 1999/.

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 extension 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. A slow temperature increase in combination with drainage through the rock implies that this is not a problem but it should be checked by calculation. If the rock is very tight, 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 large. The process is partially dealt with below (Interaction buffer/canister). Rock movements are dealt with in the process descriptions for the geosphere.
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 bentonite is eroded and carried away by groundwater.

The depth of 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 , into an ideal fracture can be estimated according to the Equation 3-15 (derived from simple integration of force equilibrium):

$$z = \frac{\delta}{2 \tan \phi} (\ln \sigma_0 - \ln \sigma_z) \quad (3-15)$$

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 approach infinity when the swelling pressure at the gel limit approaches zero. If a swelling pressure of 1 kPa is set as a limit, the penetration from a buffer with swelling pressure 10 MPa into a fracture with width 0.1 mm will be 1.3 mm if a friction angle of 20 degrees is assumed (an average). If a limiting pressure of 1 Pa is set, the penetration will be 2.2 mm. According to Equation 3-15, the penetration depth increases by about 20% for a 10 fold decrease in applied swelling pressure. Since the minimum swelling pressure in a stable gel is 0.1–1 Pa, the maximum penetration for MX-80 can be estimated to be 2.2–2.6 mm. According to Equation 3-15, the penetration depth is also proportional to the fracture width, which means that as a rule of thumb the penetration is limited to about 25 times the fracture width.

At present, a large research project is running with the purpose of investigating the penetration and loss of bentonite to fractures in deposition holes. This project is expected to yield more information. The process is also dealt with in Section 3.5.11.

The influence of the buffer on the rock is best investigated experimentally by measuring the swelling pressure on the rock at full scale. This has been done in BMT in Stripa /Pusch et al. 1985/ and in several of the full-scale tests in Äspö HRL (see e.g. /Goudarzi et al. 2003b/).

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 metre 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.

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 3.5.11.

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 porewater 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, whereas the influence of the weight of the buffer on the canister is negligible.

The mechanical interaction between buffer and canister is summarised 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.

Recent tests have revealed that a high water pressure can affect the validity of the effective stress theory in the sense that the hydraulic pressure cannot be added to the swelling pressure. The sum is instead slightly lower (only about 90% of the porewater pressure is added). This small deviation from the effective stress theory is favourable for the canister.

Another finding is that a highly compacted bentonite sample that has been exposed to very high water pressure (~30 MPa) does not resume its original swelling pressure after removal of the water pressure /Harrington and Birchall 2007/. This process and its consequences are being investigated.

2. Thermally induced porewater 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 the period of increasing temperature
2. The rate at which water volume decreases in response to the pressure reduction during drainage of water through the buffer to the rock and backfill is slower than the water volume increase caused by thermal expansion of the water during the period of increasing temperature.

Preliminary calculations have shown that the latter criterion is not probable /Pusch and Börgesson 1992/. The first criterion above may be fulfilled but is not enough on its own to cause 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 3.3.3. High gas pressures are only expected as a possible consequence of corrosion of the insert of a failed canister.

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 products have 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 is discussed further in the Canister Process Report /SKB 2010k/.

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 porewater 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-dependent 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-dependent shear deformations (deviatoric creep).

During primary consolidation after loading, the porewater pressure is the controlling 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 porewater carries the total pressure difference. With time, as the porewater pressure difference is reduced due to outflow of water, the pressure induced by the canister mass is transferred from the porewater to the clay skeleton and the clay is thus deformed. This process dominates as long as there are porewater pressure differences in the buffer.

After pore pressure equilibrium, the creep processes dominate. Volumetric creep is caused by internal microstructural reorganisation 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 dependent 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. 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/.

The latest studies of deviatoric creep /Börgesson and Hernelind 2006a/ has aimed 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 plasticisation 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 bend.

The effect on the canister depends on the stiffness or shear strength of the bentonite in relation to the stiffness of the canister. The shear strength of bentonite depends 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 thought to be small due to the small void available inside the canister.

8. Liquefaction of the buffer material

A process that could affect the canister significantly is liquefaction of the buffer. Liquefaction is a process implying that a stiff material (soil) turns into liquid due to an effect with short duration, see e.g. /Lambe and Whitman 1969/. It may take place in a loose sand when the porewater pressure is increased either due to a vibration that makes the sand particles float in the porewater (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 was 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 increases in stress will be taken up 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 result from an earthquake and requires a reduction in the 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.

Another phenomenon that could also lead to similar loss in effective stress would be the very high water pressure that may be derived from the melt water after a glaciation. However, as shown by /Harrington and Birchall 2007/ the decrease in effective stress is not high enough for the effective stress to be completely lost.

The consequences of liquefaction and subsequent complete loss in effective stress could be a settlement of the canister since the buffer would not have any shear resistance. For the reasons given, this process has been ruled out in the case of the buffer.

Model studies/experimental studies

Saturated bentonite

The swelling capacity of bentonite 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 evolutionary scenarios that are associated with volume changes in a repository. Examples of the modelling exercises include 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/m³ after water saturation and the density of the backfill was assumed to be 1,900 kg/m³ after water saturation. These values correspond to higher density in the buffer and lower in the backfill than is the case in SR-Site, (Section 2.2.1 and 2.3.1). They gave an upward displacement of about 30 cm.
- Thermo-hydro-mechanical calculations of the water saturation phase in a deposition hole with different hydraulic rock properties, done for SR 97, included the displacement of the buffer/backfill interface and movements of the canister /Börgesson and Hernelind 1999/. An average density of the buffer after saturation of 2,000 kg/m³ 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. Comparisons of calculated and measured movements and densities when canisters are loaded in deposition holes.
- Modelling of canister movements for a design with two canisters in a deposition hole. 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. In this calculation the buffer was assumed to have a high density (2,100 kg/m³ at saturation) and the backfill was assumed to be rather stiff, with a density after water saturation of 2,200 kg/m³. The calculated upswelling of the buffer was about 7 cm and the total heave of the canister (including both consolidation and creep) after 32,000 years was 3 mm.
- For a rock shear, the influence of the rock density and the rate of rock displacement has been investigated for very fast shearing /Börgesson et al. 2003/. The influence is illustrated with the following examples: At a density of 2,000 kg/m³ at water saturation, the shear strength is 1 MPa at a shear rate of $5 \cdot 10^{-8}$ m/s (4 mm/day), whereas the shear strength is 3 times higher (3 MPa) at a shear rate of 1 m/s. At a density of 2,100 kg/m³ at water saturation, the shear strength is 2.6 MPa at a shear rate of $5 \cdot 10^{-8}$ m/s (4 mm/day). The shear strength is also about 3 times higher (7.6 MPa) at this density at a shear rate of 1 m/s.
- A material model has been established to calculate the effect of rock shear on the canister and buffer. 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. 2003/. 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 for the reference case (density 2,000 kg/m³, 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 a density 2,100 kg/m³, 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/m³ in order to avoid damage to the canister in case of an earthquake.

Recently a number of additional calculations have been made in order to study further the influence of mechanical disturbances on the buffer and canister.

Canister settlement

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 /Börgesson and Hernelind 2006a/. 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, the consolidation and creep in the buffer was studied without considering the interaction with the backfill. In the other set of calculations, the interaction with the backfill was included for a backfill with the same properties as an in situ compacted mixture of 30% bentonite and 70% crushed rock. The motivation for studying the behaviour of the buffer alone was that the final choice of backfill material and backfilling technique had not yet been made so that the set of calculations simulates a backfill that has identical properties to the buffer. The 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/m³. 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/m³.

The calculations included two stages, where the first stage models the swelling and consolidation that takes place in order for the buffer to reach full 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 over 100,000 years.

Volumetric creep is not modelled, which may cause a slight underestimation of canister displacement. The reason 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 its 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 canister displacement caused by this creep will be as insignificant as the deviatoric creep.

The calculations show that 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 of 7 MPa 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 for the other case with 30/70 backfill due to the upwards swelling of the buffer. At reduced swelling pressure, settlement increases but is not more than about 23 mm at the very low swelling pressure of 80 kPa for both cases.

Figure 3-15 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. This affects the degree of mobilised shear strength, which is a critical creep parameter. A reduced friction angle will reduce the strength and thus affect the degree of mobilised 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 the same initial density and swelling pressure. At a swelling pressure of 80 kPa, the deviatoric stress at failure is only 70 kPa, which for the swelling pressure 7 MPa 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 over 100,000 years is very small and for the case of 30/70 backfill will actually result in a heave of the canister. The sensitivity analyses with reduced swelling pressure corresponding to reduced density or reduced friction angle also show that canister displacement is very insensitive to such phenomena; the total settlement will be less than a few cm even at a buffer density at saturation of 1,500 kg/m³ or at a friction angle of 0.3°.

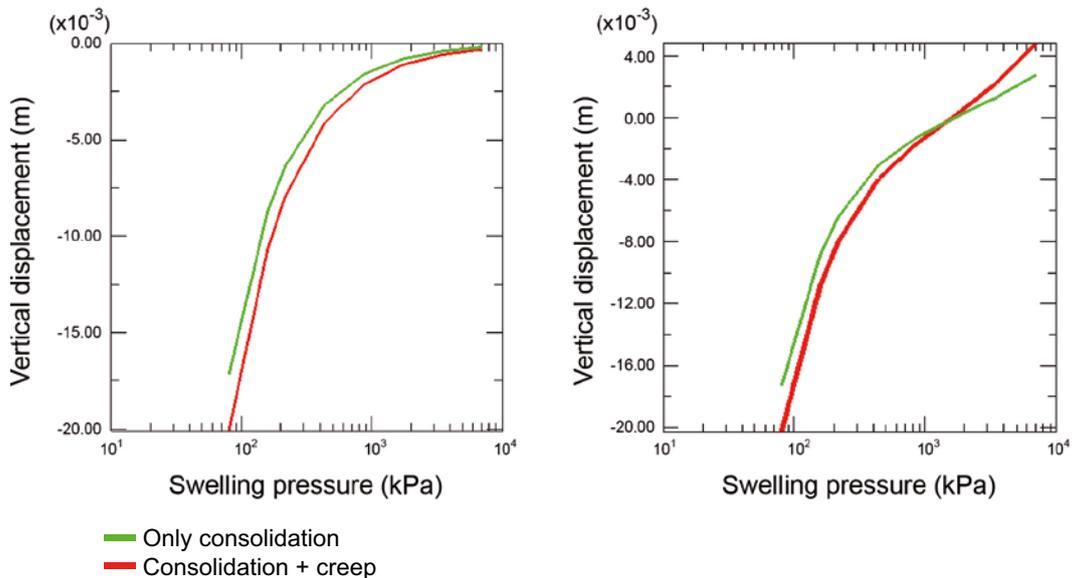


Figure 3-15. Vertical displacement of the canister as a function of swelling pressure for the two cases with fixed boundary buffer/backfill (left) and free boundary with 30/70 backfill (right). Negative displacement implies sinking /Börgesson and Hernelind 2006a/.

Rock shear

Additional calculations of the influence of an earthquake-induced 20 cm rock shear with the shear rate 1 m/s along a fracture intersecting a deposition hole in a KBS-3V repository has been done for a number of different shear cases and for different properties of the buffer material /Börgesson and Hernelind 2006b/. The influence of the following factors has been investigated:

1. Inclination of the intersecting fracture.
2. Shear direction when the fracture is not horizontal (inclination deviates from 90°).
3. Location of the shear plane when the inclination is 90°.
4. Magnitude of the shear displacement.
5. Bentonite type.
6. Bentonite density.
7. Transformation of the buffer to illite or cemented bentonite.

The results from the calculations show that all of these factors have an important influence on the damage to the canister. For most factors the influence is not easily described since there are mutual interferences. The results are further discussed below.

Plastic strain larger than 1% was reached in the copper at 10 cm shear in all cases with Na- and Ca- bentonite. However, for several cases of Na-bentonite and one case of Ca-bentonite, such plastic strain was only reached in the lid.

The plastic strain in the steel was generally smaller than in the copper mainly due to the higher yield stress in the steel.

A shear inclination of 45° was more harmful for the copper tube than a shear inclination of 90° when tension shear was considered. The highest value of the plastic strain in the copper tube was 19% and was reached after 20 cm shear in Ca-bentonite with a density 2,050 kg/m³.

At a shear angle of 90°, higher plastic strain in the copper tube was reached at eccentric shear than at centric shear for all cases except the high density Ca-bentonite case.

The maximum plastic strain in the copper tube and in the iron insert was for all cases larger for Ca-bentonite than for Na-bentonite.

Conversion to illite implies that the effect on the canister of a rock shear is insignificant compared to the case when no transformation has taken place since the stiffness and strength of the illitic clay is only a tenth of the strength of MX-80, as almost the entire swelling pressure is lost.

Cementation of bentonite to a thickness of 8.75 cm around the canister results in the effect of a rock shear being more severe than in the original bentonite due to the increased stiffness of the buffer. However, the properties of cemented bentonite are not well known so the calculation must be regarded as an example rather than as a prediction.

Additional modelling is ongoing and will be reported for SR-Site. See also the process report of the canister.

Consequences of loss of bentonite

The self healing of the bentonite buffer after loss of bentonite by e.g. erosion has been investigated in a number of FEM calculations using the basic swelling properties of the bentonite developed for Abaqus. The calculations have been performed so that part of the buffer is initially missing in an otherwise homogeneous water saturated buffer with a buffer density at saturation of 2,000 kg/m³. The results are reported in /Börgesson and Hernelind 2006c/.

The results show that the self healing properties of the bentonite are good and heal even large holes. However, friction in the bentonite prevents complete homogenisation and leaves a rather large density and swelling pressure gradient. E.g. if 121 kg is lost, the lowest resulting swelling pressure will still be higher than 1 MPa.

The extreme case of loss of all buffer material for 1 metre along the canister (corresponding to 2,400 kg dry mass of bentonite) results in the lowest estimated swelling pressure of a few hundred kPa.

Upwards swelling into a dry tunnel

If the backfill material in the deposition tunnel consists of highly compacted blocks and pellets of swelling clay instead of field compacted mixtures, the rather high swelling pressure from the block backfill prevents swelling of the buffer so that this process becomes acceptable with a high safety margin for all block types /Gunnarsson et al. 2006/. However, if the deposition hole is wet and the tunnel so dry that the buffer material becomes water saturated when the blocks are still close to the initial state there may be large displacements since there is still no swelling pressure from the backfill. This case has been investigated with some simplified calculations /Börgesson and Johannesson 2006/. The calculations yielded an estimated upwards swelling of about 8 cm. The results must be considered preliminary since the assumptions and calculation methods are uncertain and call for supplementary tests and calculations, which will be done for SR-Site and reported in the general buffer THM modelling report.

Field and laboratory tests

Experience related to swelling and homogenisation of the buffer in an emplacement borehole is available from the results of field tests in Stripa. In BMT (Buffer Mass Test), six deposition holes were simulated at 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 had achieved full water saturation in the majority of its buffer volume at the time of its excavation, which took place in the beginning of 2006. The results show that almost full homogenisation had occurred between the blocks and the pellets in the slot between the blocks and the rock surface but also that there is (as expected) a residual density difference due the friction in the bentonite.

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

- Rock shear was simulated at the scale 1:10 in three laboratory tests performed in 1986 /Börgesson 1986/. Before the shear was simulated, the bentonite was brought to complete water saturation through filters at the periphery of the buffer and the swelling pressure measured. The three tests were identical with the 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 the test was completed. The tests gave valuable information about both the effect of shear at different rates and the homogenisation of the bentonite in a deposition hole. These tests have recently been used for validating the material models and the modelling technique.
- The KBS-3H concept has also been simulated in the laboratory at the scale 1:10. Two canisters with buffer material perforated steel containers and distance plugs were installed in a tube and the swelling pressure and relative humidity RH 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 within expectations.

No heating was applied to the two tests described above.

Unsaturated bentonite

Many experiments have been conducted to study the volume change as a function of degree of saturation and void ratio under different conditions. These experiments have been used to calibrate the existing material model for unsaturated clay and to improve them.

The interaction between external stress, porewater pressure (suction) and degree of saturation in an unsaturated bentonite has been investigated in a PhD project /Dueck 2004/. This work sheds further light on the development of swelling pressure in an unsaturated buffer. A laboratory programme was run with the ultimate purpose of investigating 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. See also /Dueck 2007/ and /Dueck and Börgesson 2007/.

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 and that this is due to the fact that the rock drains the buffer. However, this calculation assumes that the rock acts as a filter for the porewater meaning that the porewater is allowed to enter the rock matrix freely.

Modelling of the Canister Retrieval Test is currently ongoing within the international project Äspö Task Force on Engineered Barrier Systems. The results from the Task Force work will be used and reported as a part of the mechanical assessment of the buffer in SR-Site. The modelling includes fully coupled thermo-hydro-mechanical simulation of the wetting and homogenisation of the buffer material. Since the test includes both unsaturated bentonite blocks with high density, a 5 cm slot filled with pellets and a 1 cm empty slot, the available mechanical models can be evaluated.

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 proportion 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 judged not 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 counteracts 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 unless lost by colloid release.
3. There will be a small remaining radial difference in density originating from the swelling of the blocks and 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 (see e.g. /Thunvik and Braester 1991/ and /Hökmark and Fälth 2003/) 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 been studied. Manmade bentonite seals are made in completely different ways (mixtures with low density) and natural bentonites have unknown histories. The existence of relevant natural analogues is probably very limited and difficult to evaluate.

Handling in the safety assessment SR-Site

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 3.3.1. Also thermal expansion and interaction buffer/backfill is included in this modelling.

Renewed calculations of the interaction between the buffer material and the new backfill consisting of blocks and pellets are done. Some results are reported in /Börgesson and Hernelind 2009/ and /Åkesson et al. 2010/.

Long-term effects

Long-term effects of ion exchange and saline groundwater are evaluated using empirical relationships described above. The effects of salinity can also be modelled by the Donnan model referred to in Section 3.5.8.

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 may 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 is high enough to prevent the formation of an expansive gel, otherwise the process has to be quantified. See further Section 3.5.11.

Earthquakes: The mechanical effects of earthquakes on the buffer will be handled in separate, integrated assessments in the SR-Site 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.

Swelling and homogenisation after loss of buffer material are modelled for SR-Site. This is a very important sub-process that extensively studied in order to improve the knowledge and modelling capability.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

The relationship between swelling pressure and density for MX-80 and Deponit CA-N and the influence of different factors are reported by e.g. /Karnland et al. 2006/. This report will undergo a documented factual- and quality review. In addition tests have been done on other bentonite types in other countries as Spain, France and Japan. An example of such a material is the Febex bentonite, which is a calcium dominated bentonite that has been used in the large scale tests in the Febex project. Results from these tests are reported in the series published by ENRESA (Publicaciones tecnicas).

The effect of canister settlement has been found to be insignificant according to /Börgesson and Hernelind 2006a/. The essential contents of this report will be transferred to the general THM report /Åkesson et al. 2010a/.

Buffer homogenisation (both natural during the saturation phase and caused by the sealing of erosion damage) and buffer upwards swelling are reported in old SKB Technical Reports but will be updated and reported in a general buffer THM modelling report that will undergo a documented factual- and quality review /Åkesson et al. 2010a/.

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. Self-healing after loss of bentonite is important and the calculations need to be checked with scale tests. Such tests are ongoing.

In the long term, swelling properties can change due to mineral transformations and cementation; see Section 3.5.9 "Montmorillonite transformation". The mechanical consequences of transformations can be assumed to lead to a higher hydraulic conductivity and a decrease in swelling pressure.

Cementation 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 3.5.9 and 3.5.6.

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

The mechanical function of water-unsaturated bentonite is difficult to model, and the models that exist today are incomplete, especially for modelling of volume change and swelling pressure. Work is ongoing and progress have recently been reached and are included in the THM report /Åkesson et al. 2010a/. 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 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 besides the behaviour in the unsaturated state concerns 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 in SR-Site

See the above heading.

Input data and data uncertainties in SR-Site

Water saturated state: Some uncertainty arises in calculating the magnitude 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, and continued validation is taking place via the field tests in the Äspö HRL and laboratory tests /Börgesson et al. 1995, Karnland et al. 2005/ some of which are ongoing . Other parameters required are fairly well known, e.g. the friction angle (which is a function of density) and the compressibility, which have an uncertainty of 10–20%. However, the friction angle at the interface between the bentonite and the rock or the canister has a special uncertainty since it depends on the roughness of the surface. Additional investigations of these interfaces will be performed.

The quality of the input data is further discussed in the THM data report /Åkesson et al. 2010b/.

Unsaturated state: Since the mechanical processes during the unsaturated period are rather poorly known, the uncertainties are large. These processes are thought 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.

3.4.2 Liquefaction

Overview/general description

This process was included in the Process Report for SR-Can. However, it has been concluded that the phenomena cannot occur in a KBS-3 type buffer material. The reasoning justifying this conclusion is discussed in Section 3.4.1. Liquefaction is no longer regarded as a process in the buffer.

Handling in the safety assessment SR-Site

Since the process cannot occur, it will not be handled in SR-Site.

3.5 Chemical processes

3.5.1 Introduction

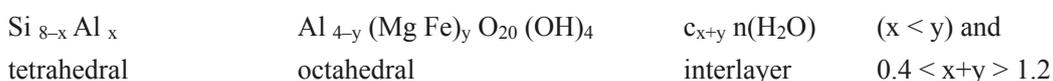
Bentonite minerals

High quality commercial bentonites normally contain over 80% montmorillonite, which means that different bentonite products have 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 lattice layer is around 1 nm (Figure 3-16) and often extends several hundred nanometres. Each layer is composed of a central sheet of octahedrally coordinated cations, which on both sides is linked through shared oxygen to sheets of tetrahedrally coordinated cations. Clay minerals of this type are often referred to as 2:1 layer structures.

By definition, in montmorillonite the octahedral sheet has aluminium as central ion, which is partly substituted, principally by magnesium and iron. The tetrahedral sheet has silicon as central ion, which may be partly substituted, principally by aluminium. 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). The structure leads to a water affinity in the interlayer space and a variable number (n) of water molecules may be incorporated between the individual mineral layers.

The ideal montmorillonite formula may be written:



and the structure may schematically be illustrated as in Figure 3-16.

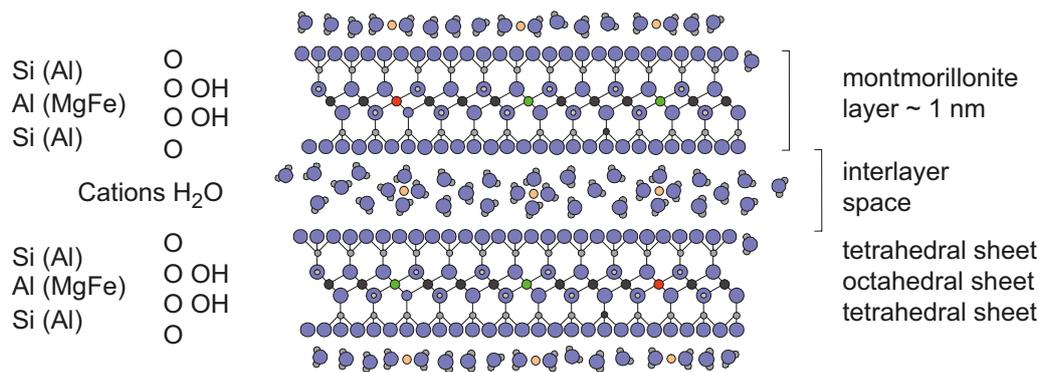


Figure 3-16. Edge view schematic of two montmorillonite layers with interlayer cations and water molecules /Karnland et al. 2006/.

Bentonite porewater

Ions in aqueous solution reduce the chemical potential and a concentration difference between solutions normally leads to water transport from the high potential (low concentration) to the low potential (concentrated) 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.

The total suction of a soil, as described in Section 3.3.1, includes osmotic suction and matrix suction. By definition, the osmotic suction is due to lowering of the chemical potential in porewater by ions, and the matrix suction refers to the lowering of the chemical potential of the porewater 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 incorporated between the individual montmorillonite layers to create an interlayer ionic solution. The cations cannot diffuse freely 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 are equal, which in the case of a pure water source theoretically leads to infinite swelling in e.g. sodium bentonite. 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, water uptake into the interlayer space will reduce the volume of initially larger pores. 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 balance the interlayer ion concentration and thereby the chemical potential in the system. The interlayer distances will thereby increase in interlayer space with high concentrations at 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 homogenisation of the pore size, due to the levelling 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 porewater 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 analysed and discussed extensively 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 inter alia the possible transport of colloids (Section 3.5.4).

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 analytically or numerically, is of major importance for equilibrium with other ions in the system, which may originate from an external solution (Section 3.5.8) or from accessory minerals in the buffer (Section 3.5.6).

The volume of a deposition hole and the corresponding buffer mass are pre-determined, and the mean interlayer cation concentration can consequently be calculated. The total pore volume in the buffer in one deposition hole is around 5,250 litres, and the bentonite mass is around 19,250 kg. The montmorillonite layer charge may be experimentally determined and is 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 charge compensating cation concentration in this system is consequently almost 3 M for monovalent ions if it is in equilibrium with pure water.

3.5.2 Advective transport of species

Overview/general description

In this context advection refers to transport of any forms of additional matter, e.g. ions, molecules or colloids, with pore-water flow. The transport direction is thereby principally from volumes of high water pressure to volumes 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, affinity for water in the bentonite and temperature induced volume change of the water. The advection is thereby closely related to water flow in the buffer, which is comprehensively described in Section 3.3.2. The advection may though be different compared to pure water flow due to ion equilibrium effects in the case of ions, and due to filtering by nano-sized pores in the case of colloids.

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

Under saturated conditions, the transport of solutes in the porewater is expected to be dominated by diffusion, see Section 3.5.3. Exceptions may be sudden events such as gas pulses or earthquakes, which can cause local pressure changes in the porewater. The improbable condition with a failure of a canister will lead to water flow into the canister due to the groundwater pressure. Corrosion of the steel insert will lead to hydrogen gas production, and the successively increasing gas pressure will reduce the inflow. The flow will stop if the water level in the canister is below the canister damage region at the time when the gas pressure exceeds the groundwater pressure. Alternatively, the flow direction will change towards the rock if the water level is above the damage. Eventually the gas pressure may reach the sum of the swelling pressure and the groundwater pressure, which would lead to a significant water flow in the latter case (See gas Section 3.3.3).

Dependencies between process and buffer variables

Table 3-9 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Site.

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 describe water transport, is available under different physico-chemical conditions, e.g. densities, salt solutions /Karnland et al. 2006/ temperatures /Cho et al. 1999/, preparation techniques /Karnland et al. 2009/ (see also Section 3.3.2).

Table 3-9. Direct dependencies between the process “Advective transport of species” and the defined buffer variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Buffer geometry	Yes, major importance before full water saturation	Included in geochemical modelling. This variable may be considered constant after water saturation	No	
Pore geometry	Yes, interlayer distance and density is a decisive parameter	Included in geochemical modelling via the parameter hydraulic conductivity	No, but indirectly, through dissolution/precipitation	Included in geochemical modelling
Radiation intensity	No		No	
Temperature	Yes, through thermal expansion and viscosity	Viscosity effect is included in geochemical modelling	No	
Water content	Yes, major importance	Included in geochemical modelling	Yes, through dissolution/precipitation	Included in geochemical modelling
Gas content	Yes, reduced flow in unsaturated clay	Neglected since the presence of gas generally will reduce advection	Yes, through transport/precipitation of dissolved gas	Neglected, since it always reduce advection
Hydrovariables (pressure and flows)	Yes, by definition	Included in geochemical modelling	Yes, minor osmotic and viscosity effects possible	Neglected
Stress state	No, Indirectly through the coupling to pore geometry	Neglected	Yes, minor effect possible	Neglected
Bentonite composition	Yes, through montmorillonite content	Included in geochemical modelling	Yes, through dissolution/precipitation	Neglected
Montmorillonite composition	Yes, minor at buffer density	Included in geochemical modelling	Yes, through ion exchange	Included in geochemical modelling
Porewater composition	Yes, by definition	Included in geochemical modelling	Yes, by definition	Included in geochemical modelling
Structural and stray materials	Potentially, as alternative transport paths	Neglected, since no stray materials are assumed to be present in the buffer	No	

The Long Term Tests of Buffer material (LOT) field test at Äspö HRL shows a total increase in ion concentration in the porewater compared to that originally present in the bentonite as a consequence of the salinity of the saturating groundwater /Karnland et al. 2000, 2009/. Precipitation of calcite and gypsum close to the central heater indicate ion enrichment and cementation (Section 3.5.6).

Natural analogues/observations in nature

Comment: Sediments rich in smectite may maintain 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-Site

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 3.5.6.

After saturation: Based on the scenario-specific evaluation of water transport under saturated conditions, process 3.3.2, advection can normally be neglected compared to diffusion. If the expected low hydraulic conductivity is for some reason not maintained, advection is included in the modelling of the canister corrosion and of radionuclide transport.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

The handling is based on the low hydraulic conductivity of the buffer material, since the resulting water flow by definition will govern advective transport. There are a large number of publications supporting the low conductivity of highly compacted sodium and calcium bentonites. The supporting reference /Karland et al. 2000/ is not peer- or factual reviewed, but it is scientifically consistent with other references that are peer reviewed articles or papers. The references /Karland et al. 2006/ and /Karland et al. 2009/ are SKB reports that presently undergo factual- and quality reviews. The references /Cho et al. 1999/ and /Karland et al. 2008/ and /Neuzil 2000/ are peer reviewed articles which are available in the open literature (Applied clay science, Physics and chemistry of the Earth, and Nature).

Handling of variables influencing this process: See process 3.3.2

Failed canister: Advective flow from the buffer 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 prevail in the buffer over timescales that could lead to significant water flow.

Uncertainties

Uncertainties in mechanistic understanding

See Section 3.3.2 for uncertainties concerning water advective transport. The magnitude of geometrical and ion equilibrium effects are uncertain but both effects will reduce the advective transport of species.

Model simplification uncertainties in SR-Site

Unsaturated conditions: see Section 3.3.1.

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 in SR-Site

Unsaturated conditions: See Section 3.3.1.

3.5.3 Diffusive transport of species

Overview/general description

Solutes can be transported in stagnant porewater by diffusion, following concentration gradients. Solutes 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 canisters. Diffusion of Na⁺ and Ca²⁺ ions is, for example, of crucial importance to ion exchange processes, diffusion of K⁺ is an important limiting factor for illitisation etc. Diffusion is central to the entire chemical evolution in the buffer.

Diffusion in bentonite has been studied thoroughly 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 3-16):

$$J = -D_p \varepsilon \frac{dC_p}{dx} \quad (3-16)$$

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

The pore diffusion coefficient D_p 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:

$$D_p = D_w \frac{\delta}{\tau^2} \quad (3-17)$$

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 3-18):

$$\varepsilon \frac{\partial C_p}{\partial t} + \rho \frac{\partial q}{\partial t} = \varepsilon D_p \frac{\partial^2 C_p}{\partial x^2} \quad (3-18)$$

Where: ρ is the bulk density of the material and q is the tracer concentration in the solid phase. For conditions where sorption is linear (i.e., not dependent on the concentration of the diffusing tracer), Equation (3-19) can be written:

$$\frac{\partial C_p}{\partial t} = D_e / (\varepsilon + K_d \rho) \frac{\partial^2 C_p}{\partial x^2} = D_a \frac{\partial^2 C_p}{\partial x^2} \quad (3-19)$$

Where: K_d is the distribution coefficient (see Section 3.5.5), D_e is the effective and D_a the apparent diffusion constant, which are defined as follows:

$$D_e = \varepsilon D_p \quad (3-20)$$

$$D_a = D_e / (\varepsilon + K_d \rho) \quad (3-21)$$

The term (ε + K_dρ) is also known as the capacity factor a of a porous medium. When sorbing solutes are present at trace levels, sorption is independent of their concentration (i.e. the concept of a linear sorption isotherm applies), and C_p can be replaced by the total concentration in the porous material, which gives:

$$\frac{\partial C}{\partial t} = D_a \frac{\partial^2 C}{\partial x^2} \quad (3-22)$$

where C is the total concentration of the diffusing ion. Equation (3-22) is the relationship that is normally used for diffusion studies of radionuclides in bentonite. For diffusion of inert, non-interacting species (implying K_d = 0 in Equation (3-22)), D_a is equal to D_e/ε.

Note that this relationship does not apply to inert anionic tracers, even though a formal K_d = 0 is typically assigned to these species. This is because the diffusion of anionic tracers through clay is influenced by the permanent negative charge of clay surfaces, which gives rise to the anion deficit/Donnan potential in clay pores (see below and Section 3.5.8). In terms of using Equation (3-21) in the context of diffusive transport of trace contaminants, the effect of anion deficit is typically handled by assigning a value to ε which is lower than the physical porosity (see section on uncertainties).

Enhanced apparent cation diffusion: It has been observed in several cases (cf. /Yu and Neretnieks 1997/) that the apparent diffusion coefficient (D_a) for cations and their respective distribution coefficient (K_d) do not correspond as expected. D_a has been higher than expected from K_d values 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 porewater 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 most 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 apparently enhanced diffusivities, which must be taken into consideration in safety assessments. The presently available information suggests that these cases are largely restricted to mobile and cationic elements: Cs, and sometimes Sr and Ra /Ochs et al. 2004/ and the SR-Site Data Report /SKB 2010/.

Enhanced cation diffusion can be explained by a cation excess in 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 3.5.8 Note that cation excess (as well as anion deficit, see below) have been well established in clay chemistry (see e.g. /van Olphen 1991/) and that the mean cation excess/anion deficit in the EDL corresponds to the differences in cation/anion concentrations in compacted clay pores as calculated through Donnan equilibrium (see Section 3.5.8).

Because these electrostatic effects increase the dissolved concentration of cations in the pore space in comparison to the corresponding (external) bulk solution and in comparison to neutral and anionic species, diffusing cationic tracers have higher concentration gradients and therefore higher diffusion rates than would be expected in the absence of the electric charge effects in the clay pores. Note that this holds for cations that accumulate in the diffuse layer, thereby retaining their mobility parallel to (but not perpendicular to) a mineral surface; but does not hold for specifically (i.e. chemically) sorbed surface species formed at surface complexation or ion exchange sites. i.e., for an evaluation of diffusive transport in compact clays, the simple accumulation in the counter-ion swarm of an electrical field near a surface and actual sorption (represented by K_d) need to be distinguished.

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 by 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 has 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 clays decreases. In compacted bentonite, the pore width is small enough to cause a superimposition of the electrical double layers between two negatively charged pore walls. i.e., the EDL's in compacted clay are truncated and no free (bulk) porewater exists /Ochs et al. 2001, 2004/. Under such conditions, the anion deficit in the diffuse layer applies to the entire pore space (see above and Section 3.5.8) and causes, for anions, the opposite effect as was explained above for cations: Diffusing anionic tracers have lower concentration gradients, and therefore lower diffusion rates than would be expected in the absence of the electric charge effects in the clay pores. An alternative view of the same phenomenon is that the anion deficit in the clay pores decreases the available diffusion pathway for an anionic tracer. Therefore, this phenomenon is often termed anion exclusion. This terminology is accepted for the present report, but it needs to be made clear that it refers to exclusion in terms of concentration (anion deficit or Donnan exclusion, see Section 3.5.8) and does not refer to exclusion due to restrictions in physical pore width. This means that the underlying concept considers a uniform physical porosity and only one type of pores in compacted bentonite /Ochs et al. 2001, 2004/, which is consistent with the concept described in Section 3.5.8.

Evidence from activation energy measurements suggests that the overlap of EDL's may occur at a dry density of about 1,200–1,500 kg/m³ /Kozaki et al. 1998/. 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/, and in sand-bentonite mixtures it is negligible. 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.

Dependencies between process and buffer variables

Table 3-10 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Site.

Influence of pore geometry: The influence of pore geometry is included by considering tortuosity and constrictivity in the equations for diffusion coefficients.

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 3-10. Direct dependencies between the process “Diffusive transport of species” and the defined buffer variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Buffer geometry	No		No	
Pore geometry	Yes	Porosity is included in the model	Possibly indirectly through influence on porewater composition and swelling	
Radiation intensity	No		No	
Temperature	Yes	Neglected for radionuclide transport – the temperature will be low when the process occurs	No	
Water content	Through pore geometry and porewater composition	(saturated conditions assumed)	No	
Gas content	No	(saturated conditions assumed)	In case of dissolved gases such as CO ₂ or CH ₄	See 3.3.1
Hydrovariables (pressure and flows)	No		No	
Stress state	Indirectly through pore geometry		Possibly indirectly through influence on porewater composition and swelling	
Bentonite composition	Indirectly through porewater composition		Indirectly through influence on porewater composition	
Montmorillonite composition	Extent of EDL depends on magnitude of charge and physical pore width	Included in data selection	Composition of exchangeable ions: indirectly through influence on porewater composition	
Porewater composition	Extent of EDL depends on ionic strength	Included in data selection	Through diffusive transport of main constituents	Included in model, see Section 3.5.6
Structural and stray materials	Through influence on physical porewidth	No stray materials are assumed to be present within the buffer	Possibly indirectly through influence on porewater composition	

Influence of bentonite/montmorillonite composition and structural/stray materials: The diffusion properties are dependent on the interlamellar space in the bentonite which 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, dissolved strontium has lower diffusivity at high concentration of sulphate, which can be explained by the formation of the neutral aqueous complex SrSO_4 /Ochs et al. 2001/. Changes in porewater composition that cause changes in ionic strength also influence diffusion 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 3.5.6.

Boundary conditions

Diffusive transport in the buffer is relevant regarding two aspects:

- Any ions or dissolved gases involved in geochemical alterations of the buffer material (as well as any corresponding reaction products) have to be transported through the buffer by diffusion.
- In case of canister failure, the dissolved concentration of most radionuclides will be limited by the formation of radionuclide-bearing solid phases, including pure solids (such as oxides, carbonates) and solid solutions. Migration of the traces remaining in solution towards the geosphere is limited by the slow diffusive transport through the buffer.

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

For 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 directly the required input parameters D_e and porosity, are largely restricted to mobile tracers (Cs, HTO, anions).

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. Further results are discussed in /Ochs and Talerico 2004/. More recently, results of through-diffusion experiments have become available especially for clay rocks (argillites) as well as some bentonites. These new data are considered in /SKB 2010l/ and are used to update the selection of diffusion parameters.

/Yu and Neretnieks 1997/ also give a detailed discussion of different experimental methods and how the results can be interpreted. For comparison 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 evaluating diffusion behaviour and for determining constants is limited due to the difficulty of determining the conditions that existed in the past. Natural analogues can illustrate that diffusive transport is greatly slowed down for many sorbing radionuclides (e.g. /Smellie and Karlsson 1996/, see also Section 3.5.5).

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 event of a defective canister, slow diffusion is very important in delaying, reducing and in many cases completely preventing releases of radionuclides.

Handling in the safety assessment SR-Site

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 alteration of impurities (Section 3.5.6). 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 3.6.1. For the treatment of radionuclide diffusion, element-specific effective diffusivities are used together with corresponding porosities (see /Ochs and Talerico 2004/ and the SR-Site Data Report /SKB 2010l/) for the definition of data and associated uncertainties).

Boundary conditions: See Sections 3.5.6 and 3.6.1 referred to above.

Influences and couplings: 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 3.5.6.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

Most general issues relevant for handling diffusion are discussed in the Section 3.5.6 and 3.6.1. All radionuclide-specific data are taken from the SR-Site Data Report /SKB 2010l/, which will undergo a documented factual review. Most of the data are based on a SKB report /Ochs and Talerico 2004/ specifically dedicated to the derivation of porosity data as well as diffusion and sorption coefficients that are consistent with the specified buffer density and composition considered in SR-Site. Sets of diffusion-available porosities and effective diffusion coefficients were selected by /Ochs and Talerico 2004/ for anions, cations (essentially Cs) and elements existing largely as neutral species (on average) under the relevant porewater conditions. To define selected parameter sets, a large amount of original experimental data, published for the most part in peer-reviewed journal articles and proceedings, was evaluated. In a follow-up peer-reviewed paper /Ochs et al. 2006/, the approach used by /Ochs and Talerico 2004/ was presented, together with a few selected datasets. /Ochs and Talerico 2004/ was also peer-reviewed according to the instructions for the SR-Can assessment.

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 any 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 EDL's.

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 effects of enhanced or diminished ion concentrations in the volume of the pore space, 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 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. On the other hand, 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-Site (SR-Site Data Report /SKB 2010/ and /Ochs and Talerico 2004/), anion exclusion is taken into account through a decrease in D_e and a reduced diffusion-available porosity. Enhanced cation diffusion is accounted for by an increase in D_e in combination with the physical porosity.

Model simplification uncertainties in SR-Site

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 3.5.6 and 3.6.1). 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 lead to a significant alteration of bentonite properties, it may be necessary to use input parameters that differ from 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 hand and C processes on the other, the present state of the art for quantifying radionuclide diffusion in compacted bentonite does not allow this. To date, semi-mechanistic models have been proposed and tested for only a few elements (Cs, Sr, anions; see above). At the same time, in the case of many relevant radionuclides there is a clear lack of systematic data from through-diffusion experiments that would be needed to further develop diffusion models in a meaningful way. Except in the case of fairly mobile elements, through-diffusion experiments often cannot be performed within a reasonable timeframe.

Whilst 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-Site. 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-Site will be similar to the conditions considered in the derivation of input data.

Input data and data uncertainties in SR-Site

Input data to SR-Site 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-Site data report.

3.5.4 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. The fundamental (dispersed in water) particle size of the bentonite is $< 2 \mu\text{m}$. 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 mean 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 homogenisation 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 homogenisation may be seen as governing variables.

Experiments with 15 nm gold colloids show that the microstructure of a bentonite with a dry density of $1,000 \text{ kg/m}^3$ effectively filters gold colloids /Kurosawa et al. 1997/, /Holmboe and Wold 2010/. This corresponds to a saturated clay density of about $1,640 \text{ kg/m}^3$. However, organic colloids will diffuse through bentonite, but the transport capacity is limited (see below).

Dependencies between process and buffer variables

Table 3-11 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Site.

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 $1,000 \text{ kg/m}^3$ 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 $1,800 \text{ kg/m}^3$.

/Wold 2003/ reports on diffusion experiments with organic colloids through MX-80 bentonite with a range of dry densities from 600 to $1,800 \text{ kg/m}^3$. 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 \AA . 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 the course of the experiment. The issue of organic colloid-related transport of radionuclides is one that warrants further examination.

/Holmboe and Wold 2010/ have performed diffusion experiments with colloids in compacted bentonite. Gold colloids are effectively filtered by compacted bentonite. Some transport of gold colloids takes place in bentonite of lower density (1.0 g/cm^3), but very slowly, see Figure 3-17.

Time perspective

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

Table 3-11. Direct dependencies between the process “Colloid transport” and the defined buffer variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Buffer geometry	No Colloid filtration is assumed to be on or off		No	
Pore geometry	Decisive importance	The lowest buffer density to facilitate colloid transport is defined	No	
Radiation intensity	No		No	
Temperature	Very minor	Excluded – No data available and temperature range will be narrow	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	Indirectly through pore geometry		No	
Montmorillonite composition	Through layer charge	The lowest buffer density to facilitate colloid transport is defined	No	
Porewater composition	Possibly a very minor effect through viscosity	Excluded	No	
Structural and stray materials	No		No	

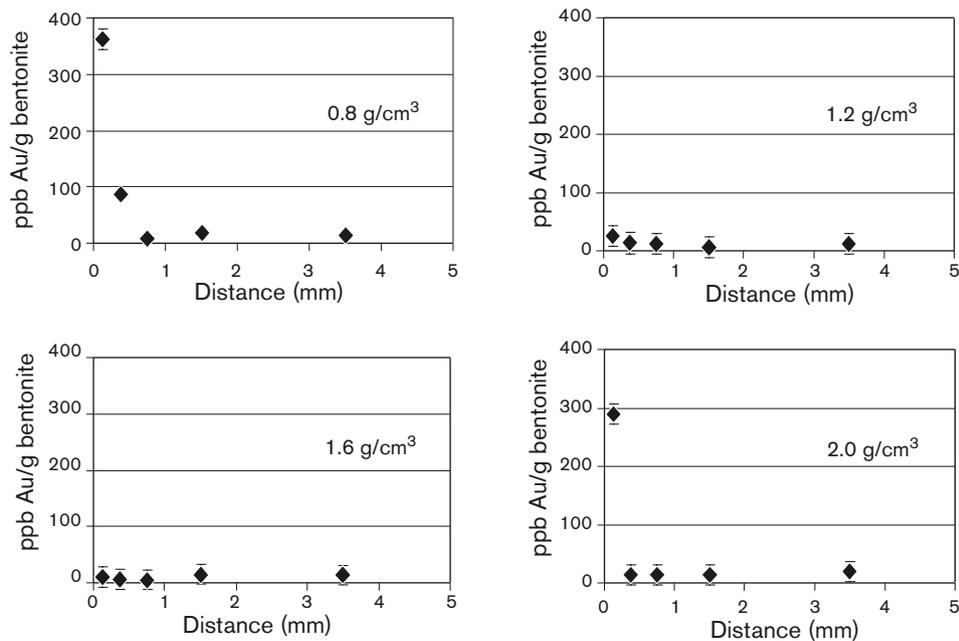


Figure 3-17. Concentration profiles of gold in the compacted bentonite pellets that were used in the diffusion experiment. The high value for the first data point in the graph, 2.0 g/cm³, is presumably the result of contamination, since the swelling pressure at the high dry density caused deformation of the metal filter /Holmboe and Wold 2010/.

Natural analogues/observations in nature

No applicable observations of the colloid filtration effect are available from nature.

Handling in the safety assessment SR-Site

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 is neglected, provided the buffer completely envelops the canister and has a dry density of at least 1,000 kg/m³, i.e. a saturated buffer density of at least 1,650 kg/m³. This is based on the experimental results from /Kurosawa et al. 1997/ and /Holmboe and Wold 2010/.

The consequence of a loss of the colloid filtration effect is treated as a separate case with transport of radionuclides in/sorbed on a colloid phase. This would mean that the concept of solubility limits is not valid. Radionuclide solubilities as well as sorption coefficients are adjusted for that case.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

/Kurosawa et al. 1997/ and /Holmboe and Wold 2010/ are peer reviewed publications. Their findings are also consistent with each other.

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 large difference between inorganic and organic colloids.

Model simplification uncertainties in SR-Site

If the buffer density is high enough to exclude colloid transport, no model is needed in the assessment. Bounding calculations can be done by adjusting input data.

Input data and data uncertainties in SR-Site

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

3.5.5 Sorption (including ion-exchange of major ions)

Overview/general description

Radionuclides and major ions in the buffer porewater 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 and also of major ions, which 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 surface, where two main types of sorption take place /e.g. Sposito 1984, Stumm and Morgan 1996/.

- The siloxane ('layer') surfaces of clay minerals are *permanently charged surfaces*. These charges derive from isomorphous substitutions, which result in a constant negative surface charge. This charge is partly compensated for by cations located at (and bound to) the clay surface (e.g. at the di-trigonal cavity /Sposito 1984/), and partly by cations simply accumulated in a counter-ion swarm. The latter is equivalent to an electrical double layer extending from the surface (see Section 3.5.1). Macroscopically, sorption takes place when compensating ions are exchanged. *Ion exchange models* of the site-binding type 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 variably charged 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 exchange 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.

The processes can be roughly divided into ion exchange and alteration of the total quantity of cations. The most important factor for both processes is the ion content of the porewater, which is principally determined by the original cations in the exchange positions of the montmorillonite, 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. Owing to its amphoteric properties, i.e. ability to both receive and donate hydrogen ions, the montmorillonite can counteract external changes in pH /Wanner et al. 1992/.

Reversibility of sorption is a fundamental paradigm with regard to

- quantitatively expressing solid/liquid partitioning of solutes through K_d values;
- the use of K_d values in transport models (for dissolved radionuclides and any other solutes).

Therefore, the available evidence for the processes relevant for radionuclide sorption to clays – surface complexation and ion exchange – is examined in the following sections.

In the absence of any evidence to the contrary, a fundamental and widely accepted principle is that cation exchange and surface complexation on clay and oxide-type minerals is reversible, which follows directly from analogies with corresponding exchange and complexation reactions

in homogeneous aqueous solutions; see e.g. /Sposito 1981, 1984, Stumm and Morgan 1996/. Accordingly, most studies concerning surface reactions on these minerals focus on sorption, whereas much fewer studies have been published that systematically investigate the degree of reversibility in sorption experiments. On the other hand, the pertinent literature offers several examples where some type of irreversibility was observed. Below, in the Model studies/experimental studies section, several examples are examined and their relevance with respect to radionuclide sorption on clays is evaluated. While this discussion is not based on an exhaustive review of the literature, it shows that sorption on clays and clay-like substrates is typically found to be reversible if the experimental boundary conditions are carefully evaluated.

Dependencies between process and buffer variables

Table 3-12 shows how the process influences and is influenced by all buffer variables.

Table 3-12. Direct dependencies between the process “Sorption” and the defined buffer variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Buffer geometry	No	(Total buffer mass is a parameter in the RN-transport model)	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	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 (CO ₂)		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/swelling	
Bentonite composition	Yes	Used for derivation of K _d	Yes	Included in geochemical transport model
Montmorillonite composition	Yes	Used for derivation of K _d	Yes	Included in geochemical transport model
Porewater composition	Yes	Used for derivation of K _d	Yes	Included in RN-transport model (Section 3.6.2) and geochemical transport model (Section 3.5.6)
Structural and stray materials	No stray materials are assumed to be present within the buffer		Indirectly through influence on porewater composition and related mineral equilibria	

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. On the other hand, the pore geometry, and thereby also the hydraulic conductivity, are not expected to be significantly altered by ion exchange processes, because the volume of the buffer at reference density is so constrained that a maximum 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/m³, 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 3.4.1 and 3.5.8).

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 number of sorption sites available 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.

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). 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/m³. 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/. This effect is mostly relevant in the case of dilute groundwaters.

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 porewater and the water in its adjacent components, i.e. the boundary conditions of the processes diffusion and advection.

Model studies/experimental studies

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

Effect of sorption/exchange processes on buffer properties: Of primary relevance for the properties of the buffer is the exchange of major cations between groundwater and bentonite pores, as well as pH-buffering by edge site protolysis equilibria. See also the process 3.5.6.

Effect of sorption on radionuclide transport: In assessing radionuclide transport from a repository, sorption is normally described as a linear, equilibrium relationship between the sorbed concentration and the concentration in solution, characterised by a distribution coefficient K_d , which is defined as:

$$K_d = q / C_w = K_d = \left(\frac{C_{init} - C_{equil}}{C_{equil}} \right) \frac{v}{m} \quad (3-23)$$

where:

C_{init} is the initial aqueous concentration of a key element [mol/m³] as measured in the reference solutions without solids

C_{equil} is the final equilibrium aqueous concentration of this element [mol/m³]

C_w is the concentration in solution

v is the volume of the solution used for a batch experiment [m³]

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 saturation), which is normally the case for radionuclides, the linear approximation is justified. K_d can also be calculated in a straightforward fashion from the output of thermodynamic sorption models:

$$K_d [\text{m}^3/\text{kg}] = \frac{\text{stoichiometric sum of surface species of element } X [\text{mol} / \text{kg}]}{\text{stoichiometric sum of solution species of element } X [\text{mol} / \text{m}^3]} \quad (3-24)$$

Surface complexation models with parameters from well-controlled experiments that include sufficient variation of key geochemical parameters can often be used to describe the dependence of sorption on external parameters such as pH, etc, see e.g. examples in /NEA 2001, 2005/.

Alkali and alkali earth element sorption to clays

With regard to the reversibility of cation exchange, /Verburg and Baveye 1994/ published a critical review of a number of studies where hysteresis (i.e., irreversibility) had been observed in cation exchange experiments. In their analysis, /Verburg and Baveye 1994/ come to the conclusion that the observed effects are related to hysteresis in clay swelling and aggregation in disperse laboratory systems (formation of quasi-crystals when the supporting electrolyte cation is changed from e.g. Na to Ca), rather than to the actual exchange process. Aggregation processes influence the exchange behaviour of clays, and their kinetics are much slower than the kinetics of exchange reactions (roughly, weeks instead of seconds).

At this point, it is important to distinguish the conditions in classical exchange experiments from those relevant for the adsorption of traces:

- The classical exchange experiments typical involve i) a complete change of the exchangeable ions (e.g., conversion of Na-clay to Ca-clay) and, concomitantly, a change of the supporting electrolyte solution (e.g. from NaCl to CaCl₂).
- On the other hand, under PA-relevant conditions, traces of a radionuclide (Sr, Cs...) are exchanged against other cations in a electrolyte solution of constant composition. Also, the exchanged trace cations do not influence the surface composition of the exchanger. In this case, no change in the clay's aggregation state has to be expected.

A somewhat special case where reversibility has been questioned is the sorption of Cs to clays. This is largely caused by a failure to distinguish between sorption on low-charge, expandable 2:1 clays (e. g. smectites) and high-charge (e.g. vermiculite) or non-expandable clays (e. g. chlorite or illite). While it is well accepted that micaceous clays, such as illite, possess so-called 'frayed edge sites' (FES) that are only accessible to few ions (Cs⁺, K⁺, protons) for steric reasons /Sposito 1984, Baeyens and Bradbury 2004/, the effect of changes in the structural properties of such clays are often not taken into account. For example, /Grütter et al. 1990/ demonstrated that sorption of Cs ions may lead (at high surface loadings) to a collapse of the interlayer of vermiculite-like clays, trapping sorbed Cs in the mineral structure and rendering desorption impossible. In the same study reversible sorption was observed at low surface loadings (i.e., where no collapse of the interlayer occurs).

There is also clear evidence that the above issues are specific to a few cations that easily lose their hydration shell and are not relevant for other ions. In an interesting study, /Cui and Eriksen 1995/ showed the reversibility of Sr(II) sorption as well as isotope exchange on several fractions of infill material (feldspar, quartz, muscovite, Fe-chlorite, probably also other Fe-minerals) from the Stripa mine, Sweden. Using reaction times between ca. 30–100 d they observed complete reversibility of Sr sorption with regard to:

- Sr concentration (no hysteresis for sorption and desorption isotherms covering 5 orders of magnitude in terms of Sr concentration);
- pH change (from pH 4 to ca. 12.5 and back);
- Sr isotope exchange.

Ni and Co sorption to clays

/Scheidegger and Sparks 1996/ examined the sorption/surface precipitation and detachment of Ni by pyrophyllite (a low-charge 2:1 clay mineral) as a function of time. Surface precipitation was presumably caused by high dissolved Ni concentrations (speciation calculations based on the thermodynamic data by /Hummel et al. 2002/ indicate that Ni was oversaturated by a factor of ca. 10 with respect to Ni(OH)₂(s), /Scheidegger and Sparks 1996/ assumed that their system was not oversaturated).

It was observed that Ni uptake was initially fast, followed by a slow process; overall equilibrium was reached after ca. 200 h (pH 7.5). The fast and slow processes were attributed to surface complexation and surface precipitation, respectively. Desorption experiments were initiated by lowering the pH from 7.5 to 6 after equilibrated samples had been stored for an additional 1–8 weeks and showed that.

- a few percent of Ni were removed within the first 2–3 h, presumably by desorbing from the surface complexation sites;
- the remaining Ni was removed much slower (based on the observed constant rate, complete removal would need about 250 days), which was ascribed to the dissolution of a Ni-surface precipitate (hypothesized as mixed Ni-Al-hydroxide);
- in comparison to experiments where the reaction products were removed every 24 h, Ni detachment was significantly slower when the reaction products were not removed, probably because of re-adsorption.

Overall, this shows that Ni adsorption onto clay surfaces is fast and reversible within similar timeframes. Similarly, /Baeyens and Bradbury 1997/ studied the sorption of trace concentrations of Ni onto Na-montmorillonite at pH 4.5–10. They report that no kinetic effects were observed for reaction times between 1 and 18 days and further state that reversibility of Ni sorption was confirmed (without giving specific data).

For Co, /O'Day et al. 1994/ observed (by EXAFS) multinuclear surface complexes of Co on kaolinite at high surface loading (just below complete monolayer coverage), whereas only mononuclear surface complexes were observed at low coverage.

Time perspective

An ion exchange process is fast, so the dissolution rate of other minerals and the transport rate in groundwater and bentonite pores will control ion exchange from Na⁺ to Ca²⁺ end member. 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: A certain cation concentration is required to compensate for the diffuse layer charge in the pore space /Ochs et al. 2004/. While the maximum concentration of Ca is limited by the solubility of calcite or gypsum, the concentration of Na is not limited, and it is doubtful that a full conversion to the Ca-form is possible under these conditions.

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 the half-life of the radionuclide, the sorption process is less important.

Natural analogues/observations in nature

Many bentonite deposits contain porewater with high salinities. Investigations of the effects of high salinity in natural smectites exist but have not been utilised 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-Site

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 3.5.6.

Failed canister: Sorption is included in the modelling of radionuclide transport for the long-term phase, see heading “Handling” for process 3.6.2. Sorption is treated through element-specific K_d values derived for specific conditions (see the SR-Site Data Report /SKB 2010/ and /Ochs and Talerico 2004/ for the definition of data and associated uncertainties).

Concerning the treatment of the fundamental assumption of reversibility, brought up at the beginning of this section, can be confirmed if:

- at least similar timeframes are considered for sorption and for desorption; but it seems that in many cases, desorption will be somewhat slower than sorption;
- there is a significant gradient or driving force for desorption (e.g. dilution, change in chemical conditions, presence of a competing sorbent), with removal of desorption products being a prerequisite for maintaining such gradients.

Exceptions to this are mainly reactions that lead to incorporation instead of sorption. For the case of clays, the main mechanism would be the collapse of certain expandable 2:1 layer structures at high surface loading. However, this is not relevant for smectite clays, due to their relatively small permanent layer charge. Based on the present information, there is no reason to assume irreversibility of sorption reactions of radionuclides on clays under relevant conditions.

Boundary conditions: See sections referred to above.

Influences and couplings: Dependence on buffer properties as well as composition and pH of the porewater in the buffer, resulting from bentonite-groundwater interaction, is considered in selecting sorption constants for radionuclide transport. Because of the conditional nature of sorption constants, the data selected 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. For the influence of ion exchange and surface acid-base equilibria on buffer chemical evolution, see Section 3.5.6; these processes are also taken into account in the derivation of radionuclide K_d values.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

Most general issues relevant for handling ion exchange of major ions and radionuclide sorption are discussed in Sections 3.5.1 and 3.5.6.

All radionuclide-specific sorption data are qualified in the SR-Site Data Report /SKB 2010/ and most data are taken from an SKB report /Ochs and Talerico 2004/ specifically dedicated to the derivation of diffusion and sorption coefficients that are consistent with the specified buffer density

and composition, as well as with the range of groundwater compositions considered in SR-Site. Distribution coefficients were calculated by /Ochs and Talerico 2004/ on the basis of porewater compositions calculated for specific bentonite-groundwater interaction scenarios. As source data for the derivation of scenario-specific distribution coefficients, a large amount of original experimental data, published for the most part in peer-reviewed journal articles and proceedings, was evaluated. For some radionuclides, calculations with thermodynamic sorption models were carried out for comparison. In a follow-up peer-reviewed paper /Ochs et al. 2006/, the approach used by /Ochs and Talerico 2004/ was presented, together with a few selected datasets. /Ochs and Talerico 2004/ was also peer-reviewed according to the instructions for the SR-Can assessment.

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 relationship 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) on radionuclide sorption, and this has to be taken into account in evaluating uncertainties of K_d values (SR-Site Data Report /SKB 2010/ and /Ochs and Talerico 2004/). In the case of some radionuclides, the underlying thermodynamic database is insufficient to quantitatively evaluate their behaviour for different conditions.

Model simplification uncertainties in SR-Site

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 a 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 the case of data selection for the SR-Can assessment using a semi-quantitative, traceable procedure to transfer K_d data from experimental to safety assessment-specific conditions /Ochs and Talerico 2004/. The same approach will be used in SR-Site. 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, provided 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 3.5.6). 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 in SR-Site

K_d values are input directly to Site for use in consequence calculations. K_d values for radionuclides for 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-Site Data Report /SKB 2010/.

3.5.6 Alterations of impurities

Overview/general description

The buffer material consists not only of montmorillonite, but also accessory minerals as well as impurities. The mineral composition of MX-80 and Deponit CA-N bentonites can be found in Section 2.2.1. In the repository environment, these accessory minerals can be dissolved and sometimes re-precipitated depending on the prevailing conditions.

The behaviour of these bentonite accessory minerals and their effect on the overall performance of the barrier depends on the interaction of groundwater with the bentonite 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 at the original site, in terms of both composition and temperature. Most accessory minerals in the bentonite are nevertheless stable in contact with the granitic groundwaters prevailing in the Fennoscandian shield. The main potential effects on the bentonite buffer are cementation of the barrier (i.e. precipitation of large amounts of accessory minerals in specific parts of the buffer), changes in the montmorillonite composition, especially the exchangeable ions that can affect the swelling capacity of the bentonite and changes in the chemical composition of porewater, which can affect the retention capacity of the near-field system.

Moreover, evaporation of incoming groundwater during the saturation phase in the warmer parts may lead to different concentrations of dissolved elements at different positions in the buffer and the consequent redistribution of accessory minerals and changes in the montmorillonite composition, resulting in an overall heterogeneous composition of the bentonite.

Another aspect of interest is the behaviour of the buffer in contact with the potential corrosion products of the cast iron insert (see Section 3.5.10 Iron-bentonite interaction). Anoxic corrosion of the cast iron insert will generate iron in solution and hydrogen, both diffusing into the bentonite. Dissolved iron entering the bentonite can precipitate as new accessory minerals (.e.g. magnetite), replace other major cations in the montmorillonite interlayer sites (cation exchange), or replace octahedral cations in the montmorillonite, which can result in montmorillonite transformation towards iron-rich clay minerals (see Section 3.5.9 Montmorillonite transformation).

Dependencies between process and buffer variables

Table 3-13 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Site.

Buffer geometry: The geometry of the buffer can affect the alteration of accessory minerals indirectly through transport of solutes in the groundwater and bentonite porewater, thus affecting geochemical reactions during its interaction. Moreover, buffer geometry determines the total proportion of accessory minerals able to react in the system due to the interaction of groundwater and bentonite.

Pore geometry: The pore geometry of the bentonite buffer affects the diffusive transport of solutes, which in turn affects the chemical composition of porewater at different points within the buffer and, therefore, the geochemical reactions taking place in the buffer. In addition, precipitation-dissolution of accessory minerals can modify the porosity distribution in the buffer as well as the pore geometry.

Radiation intensity: Only in the case of very high radiation fields; the chemical composition of buffer porewater can be modified and thus affects geochemical reactions involving accessory minerals.

Temperature: Thermodynamic constants of chemical reactions are dependent on temperature. The temperature gradient exerted by the waste canister will have a large impact on the dissolution-precipitation behaviour of accessory minerals, especially in those areas of the bentonite close to the canister. The effect of temperature on diffusion has not been considered.

Water content: The water content has an indirect effect on the alteration of accessory minerals. As the saturation process affects the transport of solutes, this in turn affects the chemical reactions. In addition, the coupled effect of temperature and saturation can result in significant changes in the redistribution of accessory minerals and on the chemical composition of buffer porewater. Precipitation-dissolution of accessory minerals can result in minor changes of porosity, and therefore the water-solid ratio or available porosity for water uptake. However, this change in porosity is expected to be very small.

Table 3-13. Direct dependencies between the process “Alteration of impurities” and the defined buffer variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Buffer geometry	Yes, the total amount of minerals in the buffer and the bentonite/ porewater ratio affects the process	The geometry and the bentonite mass, as well as the bentonite/ porewater ratio is considered in the model	No	
Pore geometry	Yes. the ratio between accessory minerals and porewater	Included in the initial conditions	Yes. Precipitation-dissolution of minerals	Variation in porosity is considered through the effect of “cementation”, which is included in the model
Radiation intensity	No	Only very high radiation fields could influence the processes	No	
Temperature	Temperature strongly influences the extent of mineral – porewater reactions	Temperature and temperature gradient is included in the chemical model	No	
Water content	Yes, could affect concentrations	The saturation phase will be considered	Precipitation-dissolution of accessory minerals modifies the porosity	The effect on the overall porosity is small and not accounted for
Gas content	An indirect 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 of gases are included in model	Yes	The results from the model are evaluated to consider effects on swelling pressure
Bentonite composition	Yes	Compositional data are considered in model	Yes	The evolution of the composition is calculated with the model
Montmorillonite composition	Yes	Compositional data are considered in model	Yes	The evolution of the composition is calculated by the model
Porewater composition	Yes	Compositional data are considered in model	Yes	The evolution of the composition is calculated by the model
Structural and stray materials	Potentially, The degradation of these materials can affect the chemical evolution of the system	No stray materials are considered in the buffer. However, effects of other system components are considered	Potentially, Secondary mineral formation/ dissolution may influence the alteration of structural and stray materials	Secondary mineral formation/dissolution is considered

Gas content: The formation of a gas phase (i.e. water vapour due to high temperature close to the canister) can modify the concentration of solutes in the porewater, and therefore the stability of accessory minerals. However, this process is only expected for the water saturation stage. Other gases are not expected to affect the behaviour of accessory minerals significantly. The formation of H₂(g) can affect the chemical evolution of the system only in the case of anoxic corrosion of the cast iron insert or other steel components in the system.

Hydrovariables (pressure and flows): Transport of dissolved chemical species in the system can modify the dissolution-precipitation rates of accessory minerals by maintaining the saturation state of these phases far from equilibrium (i.e. fast water flows around the buffer).

Stress state: Increase in the partial pressure of gases can affect the stress in the system. The build up of such partial pressures could be a direct consequence of the alteration of buffer impurities.

Bentonite composition: This is one of the most relevant variables influencing the alteration of impurities. The type and amount of accessory minerals (in addition to the montmorillonite content) determines how their dissolution-precipitation behaviour will affect the chemical evolution of the system. Moreover, the dissolution-precipitation of these mineral phases will modify the bentonite composition through their interaction with porewater.

Montmorillonite composition: The composition of montmorillonite, especially the cation exchangeable (type of cations and occupancy) is very relevant, as interaction with buffer porewater will modify the chemical composition of this porewater and, hence the dissolution-precipitation of accessory minerals in the bentonite. In addition, the alteration of bentonite impurities will modify the chemical composition of bentonite porewater and hence the montmorillonite composition.

Porewater composition: The porewater composition will determine which of the accessory minerals in the bentonite will dissolve or precipitate.

Structural and stray materials: The interaction of bentonite porewater with structural and stray materials can result in modification of the chemical composition of porewater and, therefore, in the behaviour of accessory minerals and vice versa.

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 porewater and the water in its adjacent components, i.e. the boundary conditions of the processes diffusion and advection.

The exchange of a number of solutes such as sodium and calcium ions, carbonate and oxygen is relevant to the alteration of impurities.

Model studies/experimental studies

Experimental studies regarding cementation

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/.

According to these investigations, the extent of precipitation is dependent on the temperature. At the highest temperature in the buffer (90°C), 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 had been transported to the hot iron surface, where they had precipitated. Based on a geochemical model /Pusch et al. 1993a/, it is likely 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 analysed with respect to the distribution of silica, but no definite conclusion could be drawn regarding possible enrichment in the coldest part /Pusch 1985/. 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 elemental 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) anhydrite was found in a 1–2 mm thick rim around the copper tube. The ongoing evaluation of the five-year tests /Karnland et al. 2009/ is expected to provide information on whether the precipitation is an effect of evaporation of the inflowing water as part of the saturation process, or if the process also continues after full water saturation.

Several laboratory investigations have been carried out for the purpose of studying the distribution of readily soluble ions in the pore space of the buffer after water uptake against a temperature gradient. Effects of clay density, degree of saturation, testing time, open or closed conditions, ion content and pressure in the ambient 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. Similar studies are currently being conducted in field tests at Äspö (the LOT project) /Karnland et al. 2000/ and /Karnland et al. 2009/, and in laboratory experiments under the auspices of ENRESA.

Geochemical models

There are several types of models describing bentonite – porewater interaction:

- 1) Donnan equilibrium (osmosis) models, considering the entire layer charge (CEC) to be available for influencing solution chemistry; i.e. the CEC is balanced entirely by cations in solution. Clay pores are assumed to contain no bulk water at all. See Section 3.5.8 on osmosis.
- 2) Diffuse layer (EDL) models, where the CEC is assumed to be partly compensated by cations immobilised at ion exchange sites (giving rise to sorption of alkali and alkali earth elements) and partly by ions in a diffuse layer extending from the layer surface. Bulk solution in the pores can exist at low density and/or high ionic strength /Wersin et al. 2004, Ochs and Talerico 2004/.
- 3) The ion exchange models used in the context of calculating clay alterations assume that the CEC is completely balanced by exchangeable cations. As a result, the layer surface is electrically neutral to the contacting solution, and bulk water can exist between clay platelets.

Models considering the latter case (ion exchange models) have been reviewed in this section.

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 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 direct control on calcite precipitation-dissolution, thus buffering the pH of the system. Also, the effect of protonation-deprotonation of montmorillonite edge sites can play a role in 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 will edge sites be able to buffer pH in the system. This is in agreement with experimental data obtained in the frame of the EC integrated project NF-PRO /Muurinen and Carlsson 2007, Arcos et al. 2008/, where compacted bentonite was put in contact with an external solution at high-pH and pH was measured in the bentonite at different distances from the bentonite – external water interface. The data showed that high pH values in porewater were only recorded near the interface, but pH in this zone rapidly decreased over 100 days, indicating that a chemical reaction in the bentonite is buffering the pH. Unfortunately, no information was provided on the type of reaction buffering the pH; the most likely reactions are either precipitation of calcite or protonation-deprotonation reactions on the montmorillonite surface.

The redox buffering capacity of the bentonite is more controversial. Some of the models predict that redox buffering is due to pyrite oxidation and iron (III) hydroxide precipitation; whereas other models point to iron carbonate (siderite) dissolution and iron (III) oxy-hydroxides as controlling the redox buffering capacity of the system. Experimental data obtained in the frame of the integrated project NF-PRO /Muurinen and Carlsson 2007, Arcos et al. 2008/ indicate that there is a fast and reversible redox buffering reaction occurring in the bentonite. When compacted bentonite was placed in contact with an external solution under aerobic conditions, higher Eh values were only recorded in bentonite near the contact with the external solution. Moreover, when changing the aerobic external water for another under anaerobic conditions, Eh values in the most external part of the bentonite rapidly decrease to initial values, equivalent to those in the rest of the bentonite block. These results do not allow the chemical reaction responsible for such a redox buffering effect to be identified, although the fast response of the system to changes in redox external conditions indicates that pyrite-involved reactions can be disregarded, whereas an additional process related to the oxidation-reduction of iron in the octahedral sites of montmorillonite has to be considered and investigated /Anastácio et al. 2008/.

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 with the initial conditions selected for the model. The initial conditions for the model are being revised in the framework of the LOT project.

The integrated geochemical evolution of the buffer was modelled in the SR-Can assessment /Arcos et al. 2006/. An example of the results can be found in Figure 3-18.

Natural analogues/observations in nature

Development of salt crusts in arid regions resembles in some respects certain conditions during the water saturation phase. Specific SKB-related studies have not been conducted, but a large body of literature exists on the subject. The information from these natural systems could be of interest to support information on the processes occurring during the saturation phase, as indicators of the type of minerals that can potentially precipitate in the bentonite.

Silica precipitation occurs at a large number of locations 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/.

SKB was involved in the study of a bentonite natural analogue in Spain, the BARRA Project, under the coordination of ENRESA. Two processes were studied in this natural system: 1) changes in the bentonite induced by long time exposure to a very high salinity environment, and 2) the thermal

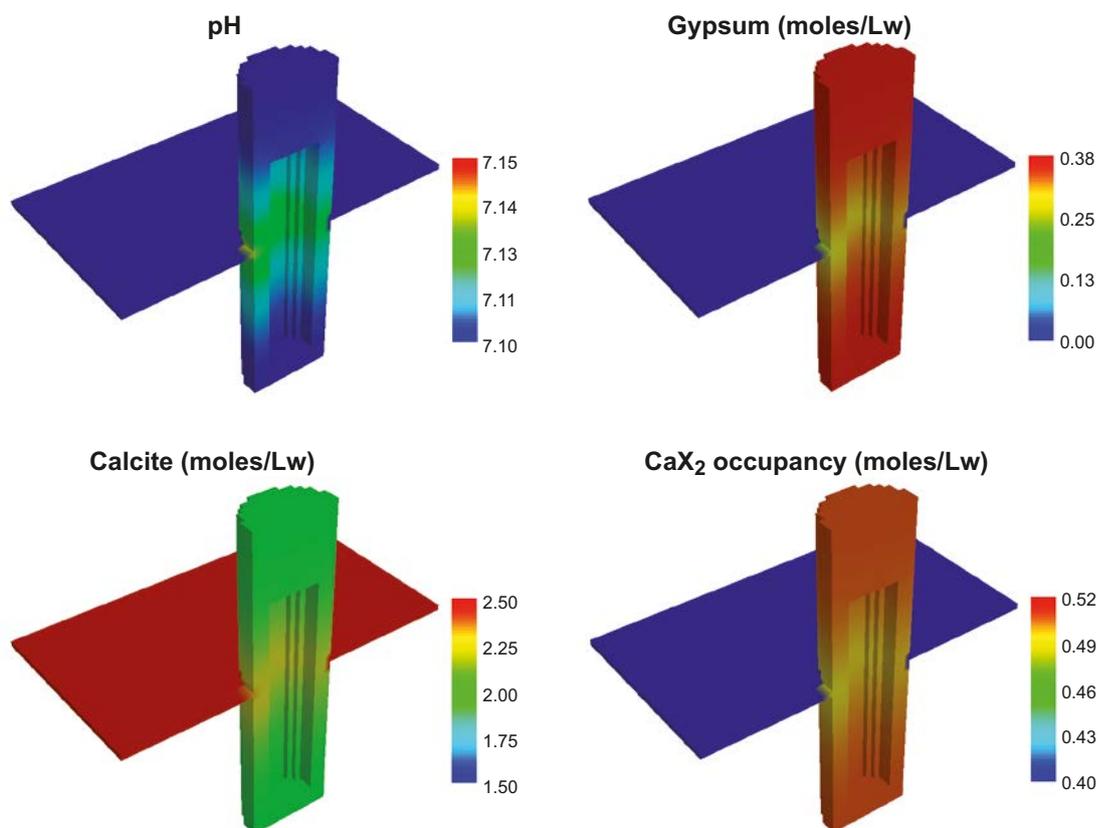


Figure 3-18. Graphics from SR-Can showing the predicted evolution in the simulated domain (Deponit CA-N bentonite) for pH, calcite and gypsum content and calcium occupancy in the cation exchanger of montmorillonite after 10,000 years of simulation. Groundwater is simulated to contact the buffer through a conductive fracture perpendicular to the deposition hole (units in moles per litre of porewater). Note that as gypsum dissolves and calcium occupancy in the exchanger is depleted calcite precipitates and pH slightly decreases /Arcos et al. 2006/

effect induced on bentonite properties by a sub-volcanic intrusion and its interaction with iron-rich fluids. The initial results from this study indicate that exposure to very high salinities does not alter the properties of the bentonite. The interaction of bentonite with iron-rich fluids at a relatively high temperature (~100 °C) resulted in changes to the smectite composition, which shifted to iron-rich members due to octahedral substitution /Pérez del Villar et al. 2005/. These studies of natural systems can give very valuable information on the long-term effect on the bentonite-porewater system of several processes that are likely to occur in the repository system, thus validating the geochemical models based on laboratory experiments.

Time perspective

Chemical precipitation/dissolution processes are likely to be most important at an early stage of repository evolution when temperature and temperature gradients are high and oxygen remains in the repository tunnels. At later stages, most of the processes approach equilibrium. The accessory minerals in the bentonite are, however, also important 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-Site

Model

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

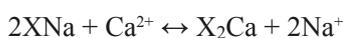
After saturation: The processes are included in the scenario-specific modelling of the buffer chemical evolution for the thermal phase and the post-thermal long-term phase. This modelling includes, in addition to alterations of impurities, the processes of diffusion (Section 3.5.3), ion exchange (Section 3.5.5), aqueous speciation and reactions (Section 3.5.7). The initial intrusion of groundwater during buffer saturation should be considered in formulating initial conditions.. The main model will be a 3D 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 the main bentonite accessory minerals, cation exchange in the bentonite, protonation-deprotonation reactions in the smectite fraction and precipitation of potential secondary phases in both bentonite and the granitic fracture. Prior to application in SR-Site, the reactive transport model was validated by comparing its results with experimental data from the LOT test.

The following is a description of the main geochemical processes considered in the alteration of impurities and how they are handled within the safety assessment SR-Site.

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 re-dissolved to some degree and then diffuse in ionic form through the buffer. Precipitation of silica may reduce the swelling potential, as well as decrease bentonite porosity.

The carbonate and pyrite contents are of decisive importance for determination of pH, Eh and alkalinity in the near field. Bentonite also contains small quantities of gypsum ($\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$), which may be of importance at an early phase during the high temperature transient.

Calcite dissolution: Calcite is stable in groundwater. In the bentonite, however, the ion exchange process will compete for free calcium ions (see also Section 3.5.5). The reaction

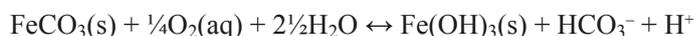


competes with



The carbonate content of the groundwaters that may be encountered is 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 redox control of the system through the following reaction



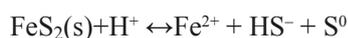
Siderite oxidation leads to an increase of iron in solution allowing the precipitation of iron (III) hydroxides and thus controlling the redox of the system. However, during the early stage, when high temperatures are expected in the buffer, hematite would be the stable iron (III) phase instead of iron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

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



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 the bentonite buffer is 12% by volume /SKB 2004/, corresponding to 1.9 moles of oxygen gas per cubic metre of bentonite, thus 0.51 moles of pyrite in 1 m³ 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 sulphide that could act as a corrodant on the copper canister. Under reducing conditions pyrite dissolves as:



The concentration of HS⁻ is an important parameter for 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 near the canister surface.

Precipitation/dissolution of silica: The main impurities in the bentonite are 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 to the canister and will be transported by diffusion outwards into the colder parts where precipitation may take place. In the Buffer Mass Test in Stripa, the buffer was analysed with respect to the distribution of silicon, but no definite conclusion could be drawn regarding possible enrichment in the coldest part /Pusch 1985/.

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 was not included in the model mentioned above, although it is envisaged to be included in the modelling in SR-Site. The reaction between iron and bentonite is also discussed in Section 3.5.10.

Boundary conditions: Main model: The diffusive transfer of species between the flowing water and the bentonite is modelled explicitly. The near-field evolution model uses the Q_{eq} 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 (porewater 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.

Changes in the accessory mineral content of the buffer 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 same as 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 of kinetic dissolution-precipitation of smectite, silica-phases and the precipitation of alternative clay minerals (kaolinite and/or illite). These scoping calculations will give some qualitative information on the relative importance of these processes and the effect on bentonite properties, e.g. porosity changes. See also Section 3.5.9.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

Most references cited are peer reviewed papers. /SKB 2004/ is a Quality Assured report. The rest of the SKB reports cited describe previous experimental studies /Karlund et al. 2000, Pusch 1985, Pusch and Karlund 1988, Pusch et al. 1992, 1998/ or models /Wanner et al. 1992, Bruno et al. 1999, Arcos et al. 2000/. Only the reference to the redox buffering process in the bentonite /Muurinen and Carlsson 2007/ has been considered for the handling in the safety assessment SR-Site. This is a deliverable from the EU integrated project NF-PRO. However, the results from this report have been published in another peer reviewed paper cited here /Arcos et al. 2008/, containing references to other peer reviewed papers on the experimental methodology.

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.

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 silica 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 for cementation as a consequence of dissolution, transport and precipitation of silica or aluminosilicate minerals. The scope and consequences of cementation cannot be predicted with reasonable certainty at present.

Finally, it is assumed that pH is buffered by equilibrium with calcite. However, the amount (or even the presence) of this mineral phase is somewhat uncertain, depending on the bentonite type selected for the buffer, thus the pH buffering capacity of the clay barrier could be affected.

Model simplification uncertainties in SR-Site

One of the major uncertainties concerns the conceptual model of the behaviour of porewater in the interlayer space of the montmorillonite. As stated previously, there are several conceptual models regarding the way the bentonite – porewater is considered (Donnan equilibrium models, diffuse layer models and ion exchange models). The effect of such different models on the geochemical evolution of the system will be evaluated.

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). One 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, which are not included in the models, as most 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 porewater, thus affecting the chemical long-term evolution of the buffer. See also Section 3.5.9.

There is no model to account 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 the hydraulic properties of the buffer. Thus, modelling of the system must 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 indication of the magnitude of these changes.

Input data and data uncertainties in SR-Site

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

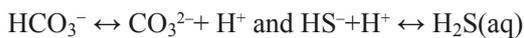
Reliable data for surface reactions (i.e. cation exchange and edge site reactions) are of paramount importance for the correct assessment of bentonite behaviour. Two types of information are needed for geochemical modelling: i) Cation occupancy of the CEC and the protonation state of the smectite surface, 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, but 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 be handled to some extent in the SR-Site data report.

3.5.7 Aqueous speciation and reactions

Overview/general description

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 porewater present at deposition, the composition of groundwater at 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 by thermodynamic and kinetic calculations. Usually aqueous speciation reactions are fast, i.e. controlled by thermodynamics. Examples are reactions such as :



Dependencies between process and buffer variables

Table 3-14 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Site.

Boundary conditions

By definition, this process takes place in the porewater. 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 in situ. The concentration 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 Section 3.5.6. Speciation of radionuclides is discussed in the process report for the Fuel and canister /SKB 2010k/ (process Speciation of radionuclides).

Natural analogues/observations in nature

Not applicable, since natural analogues are usually studied for water rock interactions and not for the water phase alone.

Time perspective

The process is important for all repository timescales.

Handling in the safety assessment SR-Site

Before saturation: Geochemical processes will be the same before and after saturation. This is just a matter of water flow and solute 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 3.5.6.

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.

Table 3-14. Direct dependencies between the process “Aqueous speciation and reactions” and the defined buffer variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Buffer geometry	Yes, the total amount of minerals in the buffer and the bentonite/ porewater ratio affects the process	The geometry and the bentonite mass, as well as the bentonite/ porewater ratio is considered in the model	No	
Pore geometry	Yes, the ratio between accessory minerals and porewater	Included in the initial conditions	Yes. Precipitation-dissolution of minerals	Variation in porosity is considered through the effect of “cementation”, which is included in the model
Radiation intensity	No	Only very high radiation fields could influence the processes	No	
Temperature	Temperature strongly influences the extent of mineral – porewater reactions	Temperature and temperature gradient is included in the chemical model	No	
Water content	Yes, could affect concentrations	The saturation phase will be considered	Precipitation-dissolution of accessory minerals modifies the porosity	The effect on the overall porosity is small and not accounted for
Gas content	An indirect 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 of gases are included in model	Yes	The results from the model are evaluated to consider effects on swelling pressure
Bentonite composition	Yes	Compositional data are considered in model	Yes	The evolution of the composition is calculated with the model
Montmorillonite composition	Yes	Compositional data are considered in model	Yes	The evolution of the composition is calculated by the model
Porewater composition	Yes	Compositional data are considered in model	Yes	The evolution of the composition is calculated by the model
Structural and stray materials	Potentially, The degradation of these materials can affect the chemical evolution of the system	No stray materials are considered in the buffer. However, effects of other system components are considered	Potentially, Secondary mineral formation/ dissolution may influence the alteration of structural and stray materials	Secondary mineral formation/dissolution is considered

Boundary conditions: See Sections 3.5.6 and 3.5.10.

Handling of variables influencing this process: The modelling is in itself a coupling of the four (groups of) processes mentioned above and 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 (porewater composition, montmorillonite composition, and bentonite composition) are also included.

Handling of variables influenced by the process: The chemical composition of the porewater is calculated. The result may have influence on the processes osmosis (3.5.8) and montmorillonite alteration (Section 3.5.9).

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

See Section 3.5.6.

Uncertainties

Uncertainties in mechanistic understanding

The model assumes that the chemistry of the porewater is identical to the chemistry in free water. The effect of the bentonite surface and structure is not included (except ion-exchange). It is not clear if or how this will affect the chemistry. See also Section 3.5.8.

Model simplification uncertainties in SR-Site

See Section 3.5.8.

Input data and data uncertainties in SR-Site

See Section 3.5.8.

3.5.8 Osmosis

Overview/general description

A classical view of osmosis, as shown in Figure 3-19, 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 permeable only to water molecules. If salt is added to the left-hand side, the water activity is reduced and transport of water from right to left will take place. The water table on the left will rise and a hydrostatic pressure develops (a). If salt is now added to the right-hand side, there will be a levelling of the water tables on both sides (b). If the initial volume change on the left-hand side is prohibited by an external force, 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 loss of pressure will evidently take place when the two concentrations become equal (d).

By analogy, assumes that the left-hand side of the system represents the bentonite buffer and the right-hand side an external groundwater solution (Figure 3-20). 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, without restriction, then the final conditions would be equal concentrations on both sides and no effect on swelling pressure would be found. Laboratory experiments show that neither of these conditions prevail and that there is a systematic reduction of swelling pressure, which indicates that ions from the external solution do pass into the clay to a certain extent /Karnland et al. 2005/.

The conditions in the bentonite/groundwater system are typical of what is often referred to as a Donnan equilibrium system /Donnan 1911/. The equilibrium is governed by the fact that some, but not all, ions can pass between the system parts, usually because of their large size. The condition

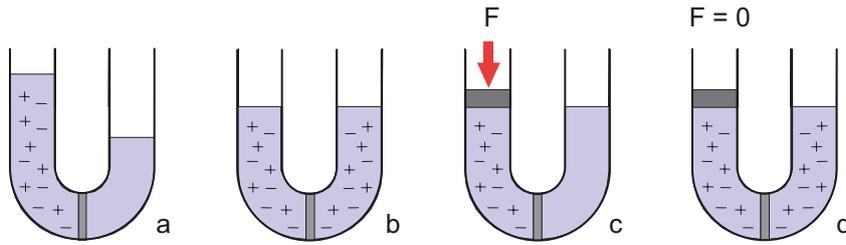


Figure 3-19. The basic principles of osmosis as an analogy of bentonite swelling pressure /Karnland et al. 2005/.

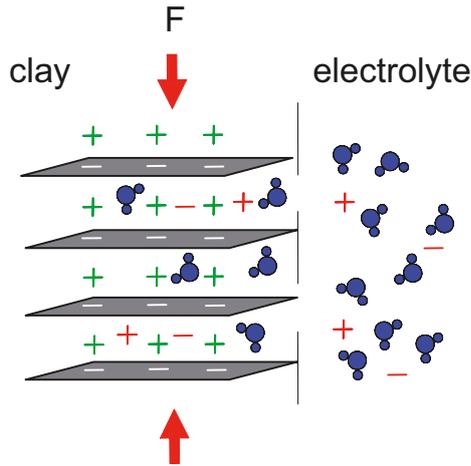


Figure 3-20. Principle drawing of the clay-water-ion system. Clay mineral flakes and charge compensating cations on the left side, and sodium and chloride ions on both sides of a semi-permeable membrane (buffer-rock interface), which is permeable to dissolved ions and water, but not to the individual montmorillonite layers /Karnland et al. 2005/.

leads to prevailing concentration differences between the two parts, including the ions which can move freely in the system. In a repository, the individual negatively charged montmorillonite mineral layers have a restricted mobility because of their relatively large size compared to the mean pore size; see Section 3.5.3 while the charge compensating cations and excess electrolyte ions may move in the bentonite/groundwater system (Figure 3-20).

The condition for equilibrium is that the electrochemical potential is equal in all system parts for all ions that can move. Since the negatively charged macro-sized mineral layers are immobile, equilibrium will be established between ions in the external solution and charge compensating cations in the montmorillonite. Ideally, for a sodium chloride solution and sodium montmorillonite these will be only Na^+ and Cl^- . The condition of electrical neutrality in the entire system is:

$$0 = z \cdot C_m + C_{\text{Cl}^-} - C_{\text{Na}^+} \quad (3-25)$$

where z is the valence of the macromolecule, C_m , C_{Na^+} and C_{Cl^-} are the concentration of the macromolecules, sodium ions and chloride ions, respectively. In terms of ion activity, the equilibrium condition for the diffusible ions is:

$$\{\text{Na}^+_c\} \{\text{Cl}^-_e\} = \{\text{Na}^+_e\} \{\text{Cl}^-_e\} \quad (3-26)$$

where the indices c and e refer to the clay-water system and to the surrounding electrolyte, respectively. The $\{\text{Na}^+_c\}$ factor is the sum of the activities of original charge compensating ions $\{\text{Na}^+_{cc}\}$ and introduced electrolyte ions $\{\text{Na}^+_{ie}\}$. The constraint of local electrical neutrality gives $\{\text{Na}^+_e\} = \{\text{Cl}^-_e\}$ and $\{\text{Na}^+_{ie}\} = \{\text{Cl}^-_{ie}\}$ which in turn gives:

$$(\{\text{Na}^+_{cc}\} + \{\text{Na}^+_{ie}\}) \{\text{Na}^+_{ie}\} = \{\text{Na}^+_e\} \{\text{Na}^+_e\} \quad (3-27)$$

Rearranging gives the introduced sodium ion activity:

$$\{Na_{ie}^+\} = \frac{-\left[\{Na_{cc}^+\} \pm \sqrt{\{Na_{cc}^+\}^2 + 4 \cdot \{Na_e^+\}^2}\right]}{2} \quad (3-28)$$

Consequently, it is possible to calculate the activity of sodium ions introduced in 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 calculated approximately if the activity of both the groundwater and the interlayer cations can be determined /Karnland et al. 2005/. Figure 3-21 shows measured and calculated results for the above conditions assuming an activity coefficient of unity. 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 to sodium.

Dependencies between process and buffer variables

Table 3-15 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Site.

Boundary conditions

The process occurs at the interface between the bentonite and an external solution, mainly the rock/bentonite interface, but could also occur at the bentonite/canister interface in the case of a defective canister.

Model studies/experimental studies

The first preliminary study concerning influence of external groundwater salinity on swelling pressure was reported in /Karnland et al. 1997/. A comprehensive model and experimental study of MX-80 bentonite converted to a pure sodium state has been made by SKB /Karnland et al. 2005/. An additional experimental study of the two reference bentonites MX-80 and Deponit-CaN in their natural state and after conversion to pure sodium and calcium forms has been made by SKB /Karnland et al. 2006/.

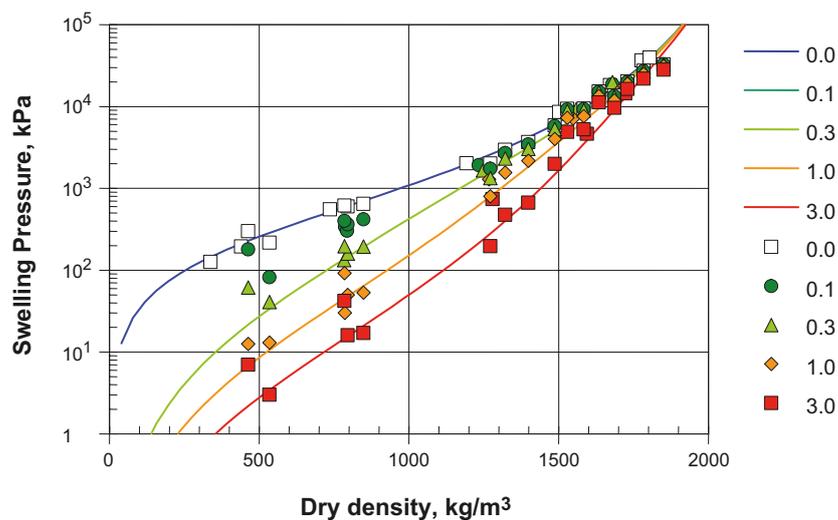


Figure 3-21. Measured (symbols) and calculated (lines) swelling pressure versus dry density of clay for different concentrations of a NaCl solution in equilibrium with Na-montmorillonite. Legends show external solution concentration in mol/dm³/Karnland et al. 2005/.

Table 3-15. Direct dependencies between the process “Osmosis” and the defined buffer variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Buffer geometry	No		No, but indirectly through stress state	
Pore geometry	Yes, interlayer distance is a decisive parameter	Included as a function of buffer density	No, but indirectly through stress state	
Radiation intensity	No		No	
Temperature	Yes, linear dependence	Neglected due to small variations	No	
Water content	Yes, equivalent to pore geometry in saturated buffer	The buffer is assumed to be saturated for this process	No, not at high buffer densities	
Gas content	No, the process is not well defined in unsaturated buffer		No	
Hydrovariables (pressure and flows)	No, but indirectly through porewater composition		Yes, hydraulic conductivity effects	The effect of salinity on hydraulic conductivity is evaluated
Stress state	No, but indirectly through charge compensating cation concentration (montmorillonite composition)		Yes, by definition	The effect of salinity on swelling pressure is evaluated
Bentonite composition	Yes, through montmorillonite content	Included in data	No	
Montmorillonite composition	Yes, through type and number of charge compensating cations	Included in data	Yes, counter-ion distribution	Ion-exchange is considered
Porewater composition	Yes, by definition	Included in data	Yes, by definition	Included in data
Structural and stray materials	No		No	

Time perspective

The process is relevant for all timescales over the lifetime of the repository. The swelling pressure response of a change in groundwater salinity is expected to be instantaneous.

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 induced pressure effects are discussed in /Neuzil 2000/.

Handling in the safety assessment SR-Site

The osmotic swelling pressure effects are handled by direct application of empirical data for relevant, scenario-specific conditions.

Model: The relationship presented above may 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 are measured for all relevant conditions.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

The principles for osmosis, ion equilibrium (Donnan equilibrium) and the resulting pressure effects are basic knowledge in physical chemistry, and are consequently supported by numerous peer reviewed articles available in the open literature. The application to bentonite buffer systems is shown in /Karlund et al. 1997/. Both are SKB reports and the latter undergo documented factual- and quality review at present. /Karlund et al. 2005/ is not an SKB report, but is developed within the framework of a quality assurance system that requires a documented factual- and quality review before approval and printing and is available in the open literature. The natural analogue support for osmosis /Neuzil 2000/ is a peer reviewed article (Nature) that is available in the open literature.

Uncertainties

Uncertainties in mechanistic understanding

The process is based on well-established theories and generally well understood. However, detailed treatment of ion activity in the buffer is not clear.

Model simplification uncertainties in SR-Site

The ion equilibrium model for predicting swelling pressure is based on the assumption that the system is relatively homogeneous with respect to pore geometry. This assumption is strongly supported by comparison of calculated and experimental data for swelling pressure, freezing (Section 3.2.2.) and tracer diffusion (Section 3.5.3).

Input data and data uncertainties in SR-Site

The input data to the model are 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 of groundwater and standard methods may be used for calculating this activity. The relevance of calculating the activity of interlayer ions by standard methods (Debye-Hückel, Davis, Pitzer etc) is not obvious. Uncertainties still remain as to how this activity should be treated in a relevant way.

3.5.9 Montmorillonite transformation

Overview/general description

The advantageous physical properties of the buffer, principally swelling pressure and low hydraulic conductivity, are determined by the capacity for water uptake between the montmorillonite layers (swelling) in the bentonite, see Sections 3.3.2 and 3.4.1. Montmorillonite can transform into other minerals (Figure 3-22) of the same principal atomic structure but with less or no ability to swell in contact with groundwater. The transformation processes usually consist of several basic mechanisms. At the physico-chemical conditions expected in a repository, the following possible mechanisms have been identified.

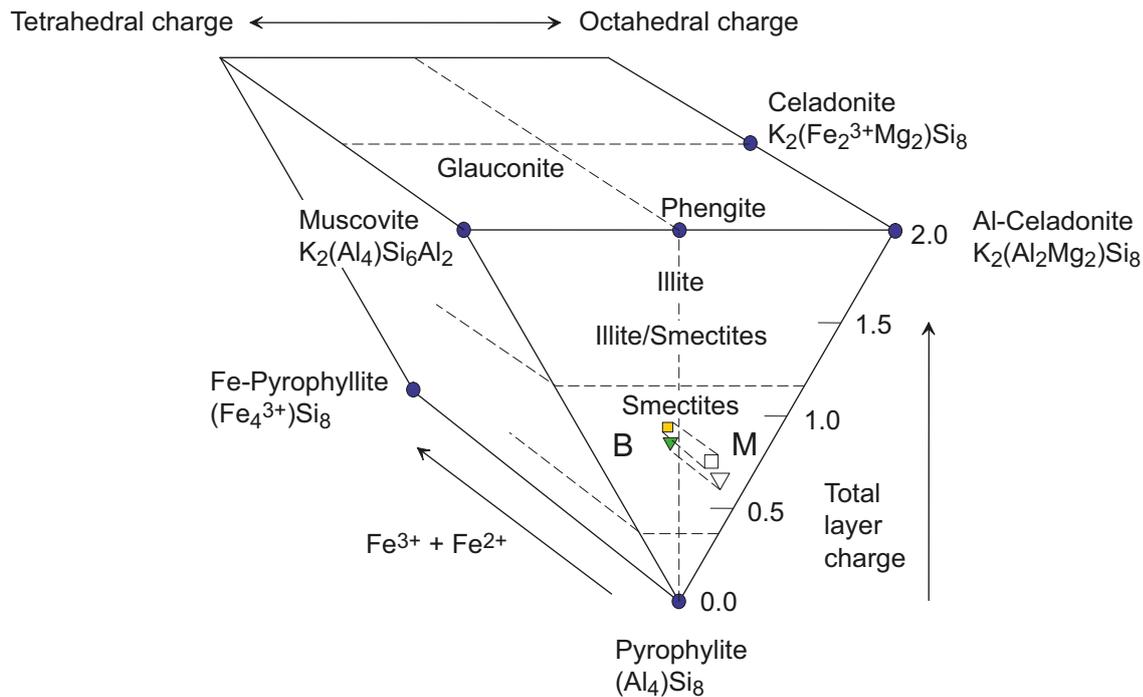


Figure 3-22. Ideal end-member minerals in the pyrophyllite – mica series with potassium as charge compensating cation, and approximate compositional ranges for illite and smectite (modified from Newman and Brown 1987). B denotes beidellite, M denotes montmorillonite. The compositional positions of the montmorillonite minerals in the reference bentonite materials are indicated by a triangle (MX-80) and by a square (IBECO RWC). All formulae contain the basic $O_{20}(OH)_4$ unit.

Congruent dissolution

Montmorillonites will not necessarily be in chemical equilibrium with repository groundwater (Figure 3-23). As mineral solubility is low, no significant mass loss is expected from this mechanism. However, solubility is temperature and pH dependent (Aagard and Helgeson 1983/).

Reduction/oxidation of iron in the mineral structure.

This process alters the layer charge and may destabilize the mineral structure (Stucki et al. 1984/). Corrosion of metallic iron or bacterial activity (Kim et al. 2004/ could promote the process (see Section 3.5.10).

Atomic substitutions in the mineral structure.

This process alters the layer charge by e.g. Al replacement of Si in the tetrahedral sheets, or Al replacement by Mg.

Octahedral layer charge elimination by small cations.

At high temperatures, e.g. Li^+ may penetrate into the octahedral sheet, which reduces the layer charge (Greene-Kelley 1953/).

Replacement of charge compensating cations in the interlayer.

Substitution of counter ions is referred to as exchange and is treated elsewhere (see ion exchange process 3.5.5). Due to charge balance, any mechanism which alters the layer charge must be compensated by addition or removal of counter ions in the interlayer. Such compensation is fundamentally coupled to processes governing transport in the porewater, see diffusion, 3.5.3.

Transformation from montmorillonite to illite, which is the most common alteration observed in natural sediments, is well documented in different geological environments, and has been reproduced under laboratory conditions. The illitization process may be seen as the first step in a transition from

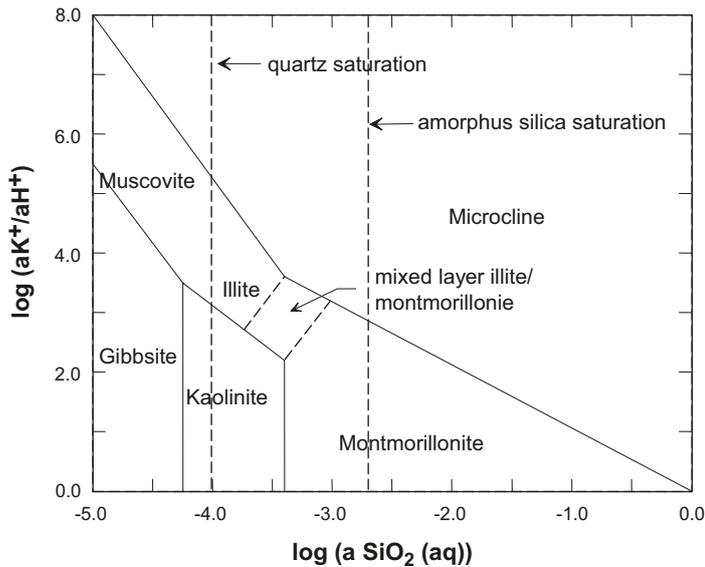
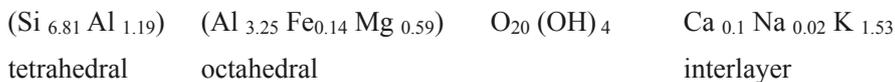


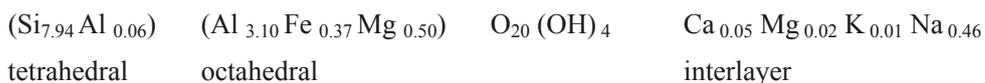
Figure 3-23. Silicate mineral equilibria with the partial component potassium at 25°C (Simplified from /Aagard and Helgeson 1983/).

montmorillonite to mica (muscovite/celadonite) minerals (Figure 3-22), and all intermediate stages from swelling to non-swelling material may be found (mixed layer smectite-illite). The conversion always involves a layer charge increase, mainly due to a decrease in silica content, and an uptake of charge compensating potassium ions. However, there is no general consensus concerning the detailed mechanisms in the conversion, and several models have been proposed.

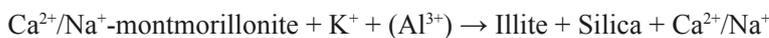
Advanced illite replacement may be illustrated by the mineralogical composition of a natural illite from Montana, US, with less than 10% swelling layers /Hower and Mowatt 1966/:



This illite mean structural formula can be compared with the mean structural formula for the montmorillonite in the MX-80 SR-Site reference bentonite /Karnland et al. 2006/:



The main mineralogical differences are that illites have approximately one unit higher tetrahedral charge, and potassium as the main charge compensating cation. Simplified, the total illitization reaction may be expressed:



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 silicate minerals. The total reaction rate is governed by the slowest of the sub-reactions.

According to the equilibrium conditions for 25°C (Figure 3-23), montmorillonite may be thermodynamically stable for silica activities above $6 \cdot 10^{-4}$. Amorphous silica, with an equilibrium activity of around $2 \cdot 10^{-3}$ may consequently be in equilibrium with montmorillonite. However, quartz with an activity of $1 \cdot 10^{-4}$ will not be in equilibrium with montmorillonite. Precipitation of quartz may therefore destabilize the montmorillonite, and the precipitation rate may be the kinetically controlling mechanism in illitization of montmorillonite /Abercrombie et al. 1994/. Figure 3-24 shows the decrease in silica activity in sediment porewater, as a function of temperature (depth in the sediments).

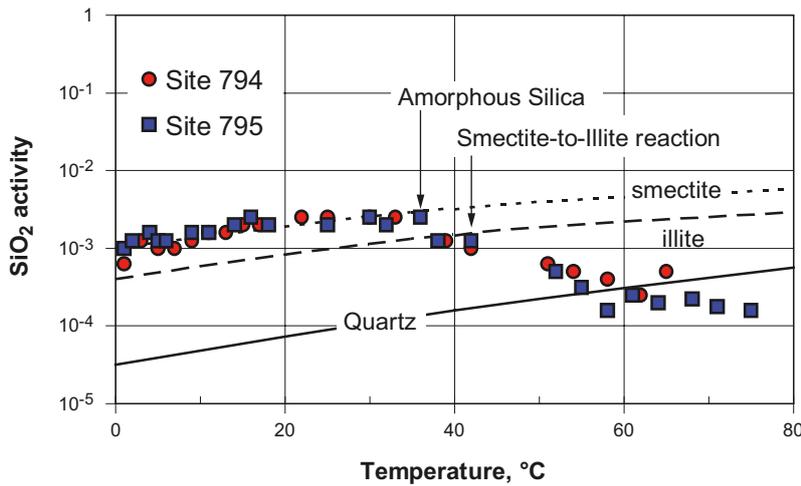


Figure 3-24. Silica activities for waters from Ocean Drilling Program sites 794 and 795 and saturation curves for amorphous silica, smectite-to-illite reaction, and quartz. Modified from /Abercrombie et al. 1994/.

At temperatures below 40°C the porewater is in equilibrium with amorphous silica, and at temperatures higher than 60°C the porewater is in equilibrium with quartz. The onset temperature of quartz precipitation in this system should consequently be in the range 40 to 60°C.

However, at low temperatures the precipitation of quartz is very slow and the porewater may stay strongly supersaturated with respect to quartz. Consequently, a high smectite content is commonly found in old formations exposed to repository temperatures. For example, /Velde and Vasseur 1992/ studied the time-temperature distribution of illitization in seven deep wells in four sedimentary basins in the US, Japan and France. In all wells there was a typical reduction of smectite content with depth, which represents an increase in both age and temperature (Figure 3-25). The prerequisites for transformation are obviously present in the sediments with time and temperature the governing parameters. A decrease to around 60% smectite was observed in the Californian Norwal formation after 4.5 million years at a depth of 5 km, representing a final temperature elevation of over 100°C. The same transformation took around 60 million years at a depth of 2 km and a temperature elevation of around 70°C in the Texan Peeler sediments. The reaction rate at these repository relevant temperatures is consequently very slow in relation to the timescale of a repository.

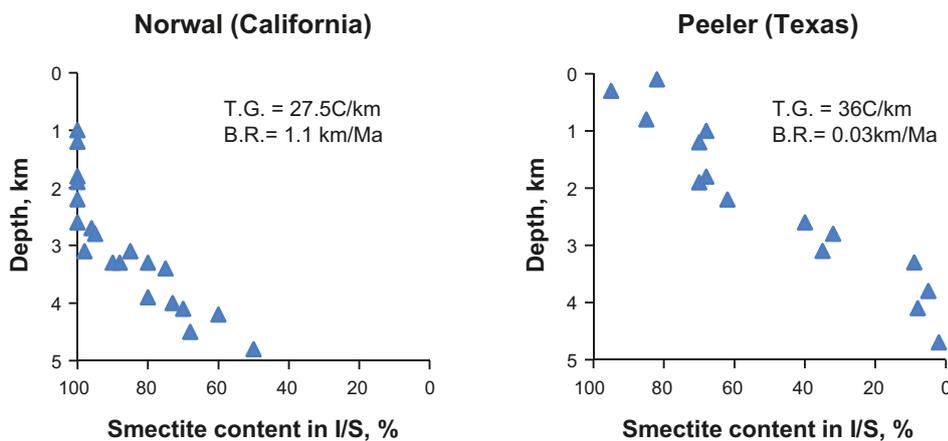


Figure 3-25. Smectite content versus depth in smectite-illite mixed layer material in two sediments representing relatively fast burial rate (left) and slow burial rate (right). T.G: indicate the present temperature gradient and B.R. indicates the burial rate. Redrawn from /Velde and Vasseur 1992/.

Brammallite/rectorite may be seen as a sodium equivalent to illite. The mean layer charge is higher than in illite, normally close to 2 unit charges per $O_{20}(OH)_4$. It is expected that the transformation from montmorillonite into brammallite/rectorite is governed by the same basic mechanisms as in illitization. The release of silica from the montmorillonite may theoretically continue until the required tetrahedral charge is reached in the absence of potassium. In consequence, brammallite/rectorite are less commonly found as alteration products in natural sediments compared to illites, and there are no indications that the basic mechanisms should be faster than in illitization.

Chlorites have the same basic structure as montmorillonite, but the layer charge is normally close to 2 unit charges per $O_{20}(OH)_4$. The layer charge is balanced by positively charged, octahedrally coordinated, hydroxide sheets, where the central ion may be any di- or tri-valent metal ion, normally Mg, Al or Fe. Transformation from montmorillonite to chlorite is occasionally found in parallel with illitization, and it is expected that both transformations are governed by similar basic mechanisms. It cannot be excluded that chlorite may be formed from montmorillonite without illitization in the absence of potassium, but there are no indications that this process would be faster than the illitization process under repository conditions.

Silica solubility increases significantly above pH 9 due to the H_4SiO_4 -species losing one or two of its protons. The total equilibrium SiO_2 concentration ($[H_4SiO_4] + [H_3SiO_4^-] + [H_2SiO_4^{2-}]$) is given by the law of mass action:

$$[SiO_2]_{TOT} \approx \{H_4SiO_4\} (1 + K_1/\{H^+\} + K_1K_2/\{H^+\}^2)$$

where $K_1 = 10^{-9.9}$ and $K_2 = 10^{-11.7}$ denote the equilibrium constants for the dissociation reactions. The total SiO_2 -concentration as a function of pH is shown in Figure 3-26, assuming an H_4SiO_4 activity for saturated amorphous silica.

The tetrahedral silica in the montmorillonite consequently equilibrates at higher concentrations above pH 9. Diffusive removal of silica or precipitation of new silica minerals thereby lead to a faster increase of the tetrahedral layer charge compared to near neutral conditions. The corresponding increase in concentration of charge compensating cation leads to a change in the interaction with water and thereby to a change in sealing properties. The layer charge may reach the critical value for collapse, which results in total loss of expandability and in principle, to the same consequences as for illitization. Eventually, the process may lead to a general dissolution of the montmorillonite /ECOCLAY II/, /Karnland et al. 2005/.

At pH 11, the divalent anion $H_2SiO_4^{2-}$ starts to play an important role leading to a dramatic increase in silica solubility. At pH 11 the total silica concentration is calculated to be approximately 16 times greater than at neutral pH conditions, and at pH 12.4, representing matured Portland cement, the theoretical increase in total silica solubility is more than 3 orders of magnitude higher than at near neutral conditions. The total difference in silica concentration between the bentonite porewater

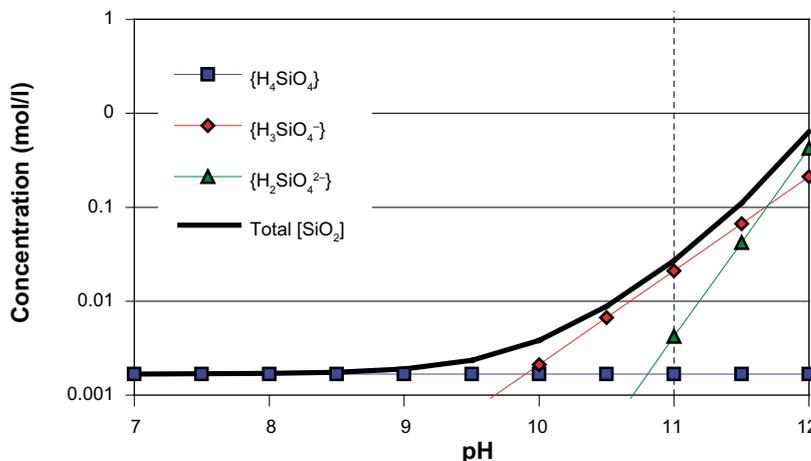


Figure 3-26. Total concentration of silica as a function of pH assuming H_4SiO_4 activity for saturated amorphous silica at 25°C. At pH=9.9 $H_3SiO_4^-$ starts to dominate and above pH=11.7 $H_2SiO_4^{2-}$ dominates. The upper limit for the KBS-3 design criterion, pH=11, is indicated /Karnland et al. 2006/.

and the groundwater increases approximately by the same factor, assuming the groundwater is in equilibrium with quartz. This leads to diffusional transport of aqueous silica from the bentonite into the groundwater. Besides the difference in equilibrium concentration, the limiting factors for this mass loss will likely be the contact area between the buffer and the groundwater and the groundwater flow. /Huertas et al. 2005/ studied the dissolution rate of smectite as a function of pH. Figure 3-27 plots log dissolution rate vs. pH at 25, 50, and 70°C. In alkaline solutions, the smectite dissolution rate increases as pH increases, showing a steeper slope for pH values higher than 11, which seems to be a critical value for smectite dissolution and stability. The conclusion from /Huertas et al. 2005/ is that the results indicate that dissolution rates are strongly affected by both pH and temperature. This effect is particularly important for pH values above 11. The effect of the alkaline plume should be especially strong for young cement waters and for a repository concept in clay rocks, where the voussoirs surrounding the bentonite are closer to the canister than the concrete plug in the granite concept, and therefore subjected to higher temperatures. In cooler regions and slightly alkaline solutions, the bentonite components should be much more stable.

Effects of montmorillonite transformation

If montmorillonite transformation occurs the buffer functions will alter. Layer charge changes in the montmorillonite lead to changes in the interplay with water and thereby affects the swelling pressure. During the early stages of illitization and similar transformations, montmorillonite/water interaction may become stronger due to moderate layer charge increase. However, as the transformation progresses, fixation of K^+ between sufficient highly charged layers leads to loss of interaction with water. The pore geometry is thereby changed towards fewer and larger pores, which in turn leads to a successive general deterioration of the buffer properties. A total transformation of all the montmorillonite in the buffer into illite or similar minerals would lead to complete loss of buffer function.

Many transformation processes and also congruent dissolution of the montmorillonite mineral releases solutes which could precipitate as new minerals which may act as cementing agents. Cementation could be enhanced due to transport of material from high solubility to low solubility regions, in situations where a solubility gradient prevails across the buffer, e.g. due to temperature and pH differences, /Karnland and Birgersson 2006/. For instance, in the case of silica, solubility increases dramatically at pH above 11 due to deprotonisation. Cementation may lead to a deterioration of the buffer's rheological properties as well as decreased capacity to swell, but these effects are expected to be small since montmorillonite transformation is expected to be minor (see Section 3.5.15).

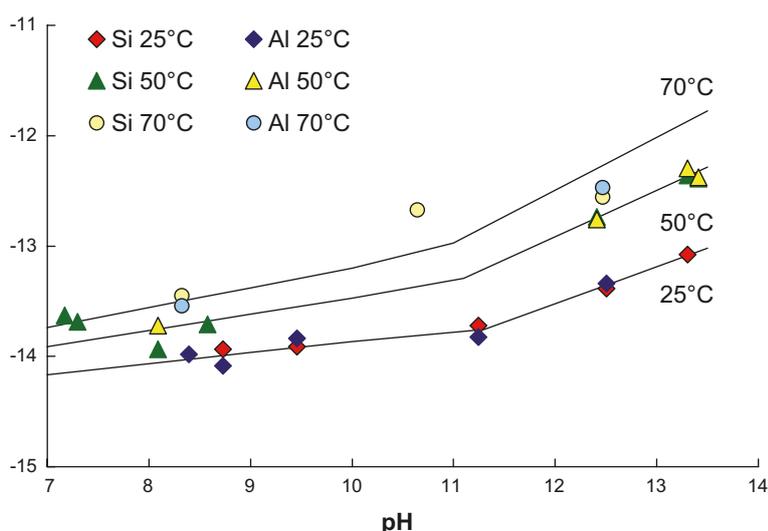


Figure 3-27. Experimental (symbols) and estimated (lines) dissolution rates /Huertas et al. 2005/.

Table 3-16 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Site.

Boundary conditions

The relevant boundary conditions for the buffer are temperature and solute concentrations in the adjacent components, i.e. the same boundary conditions as for the processes heat transport, diffusion and advection.

Model studies/experimental studies

The illitization process is of great commercial importance in connection with prospecting and extraction of oil deposits which has led to very extensive research since the 1960s.

Table 3-16. Direct dependencies between the process “Montmorillonite transformation” and the defined buffer variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Buffer geometry	Yes, the size affects the transport of dissolved species and total buffer mass	Total mass considered. Transport resistances are pessimistically neglected	Yes, for extreme (unexpected) transformation	Separate scenario
Pore geometry	Yes, the density will affect the transport of dissolved species and ion equilibrium	A kinetic expression is used. Transport resistances are pessimistically neglected	Yes, by definition	Separate scenario
Radiation intensity	Possible minor effect	Neglected, see 3.5.12	No	
Temperature	Yes, major impact	A kinetic expression is used.	No	
Water content	Yes, direct effect on hydraulic conductivity	Irrelevant for the time-frames considered	Yes, for extreme (unexpected) transformation	Separate scenario
Gas content	Yes, direct effect on hydraulic conductivity	Irrelevant for the time-frames considered	No	
Hydrovariables (pressure and flows)	Yes, minor through transport of dissolved species	Transport resistances are pessimistically neglected	Yes, major impact	Separate scenario
Stress state	No, pressures are too small to be significant		Yes, major impact	Separate scenario
Bentonite composition	Yes, through available species in accessory minerals	Minor importance, included in the assessment of effects of cementation	Yes, by definition	Separate scenario
Montmorillonite composition	Yes, by definition	Included in assessment	Yes, by definition	Separate scenario
Porewater composition	Yes, by definition	Included in the assessment of effects of cementation	Yes, by definition	Minor change that has little impact on performance
Structural and stray materials	Yes, indirectly through dissolved species. Especially pH effects from cement	Neglected in this case, since no stray materials are assumed to be present	No	

Kinetic models have been developed for the 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, Velde and Vasseur 1992, Huang et al. 1993/. Most models take 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 3-30:

$$-dS/dt = A \cdot [K^+] \cdot S^2 \cdot \exp(-E_a/RT), \quad (3-30)$$

where S is the smectite fraction in the illite/smectite material, A is the frequency factor, E_a is the activation energy, R is the universal gas constant, and T is the temperature. After integration of Equation 3-30 the smectite content at a certain time can be calculated if the temperature and potassium concentration in the porewater are known. The potassium concentrations in the Äspö groundwater have been measured and found to be in the range of a few ppm up to 45 ppm /Laaksoharju et al. 1995/. According to the model, practically no clay conversion is possible in a KBS-3-type repository under these conditions as shown in Figure 3-28.

The mineralogical stability of montmorillonite is being studied by SKB in the Lot tests at Äspö HRL /Karnland et al. 2009/. The test series represents both anticipated repository and adverse conditions. The latter are used to accelerate possible degradation processes by use of:

- Higher temperature.
- Higher temperature gradient.
- Higher content of accessory minerals (calcite, gypsum, K-feldspar).
- New substances (Portland cement).

At the highest temperature (~130°C), a test period of 10 years corresponds to the entire period of elevated temperature in a KBS-3 repository with respect to illitization according to the Huang model. The introduction of additional substances and increased temperature gradients is made in order to accelerate mass transport processes. The effect of the temperature gradient is, however, not possible to describe in a simple and generalised way by means of increased temperature and concentrations of reactants. No mineral transformation to illite has been detected in the tests performed at standard or adverse conditions by use of standard clay mineralogical analyses, nor has any K^+ -fixation been observed by the performed mineralogical and chemical analyses.

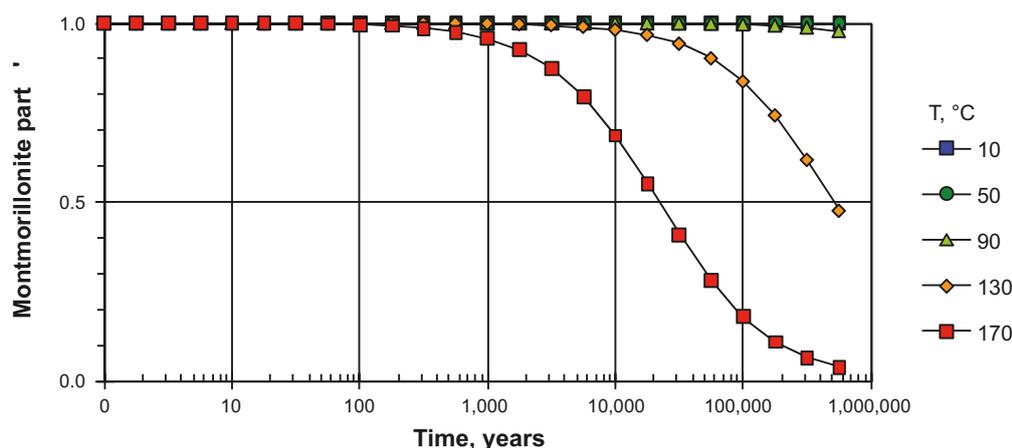


Figure 3-28. Remaining smectite fraction for different temperatures in a hydrothermal system with $[K^+] = 0.0012$ mol/liter (45 ppm) according to the Huang et al. kinetic model and laboratory determined constants ($E_a = 28$ kcal·mol⁻¹ and $A = 8.08E4$ L·s⁻¹·mol⁻¹) /Karnland and Birgersson 2006/. Legend shows temperature in °C.

Natural analogues/observations in nature

Apart from SKB-related investigations, the transformation of smectite to illite is well-documented in a large number of geological formations. Natural sediments have been studied by, among others, /Burst 1969, Perry and Hower 1970, Hower et al. 1976, Colten-Bradley 1987, Velde and Vasseur 1992, 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 a kinetically controlling factor has been studied in sediments /Abercrombie et al. 1994/. Formations where temperature effects have been obtained from e.g. volcanic activity have revealed a similar transformation /e.g. Pytte 1982, Lynch and Reynolds 1985, Brusewitz 1986/. Cementation is a consequence of montmorillonite transformation (see Section 3.5.15).

Time perspective

Reduction/oxidation reactions of iron may take place on a short time scale. Montmorillonite layer charge changes and associated precipitations may take place during the initial elevated temperature phase. Changes in montmorillonite content are relevant for the whole life-time of the repository.

Handling in the safety assessment SR-Site

The montmorillonite transformation in a KBS-3 repository is assumed to be small based on the following observations and arguments:

1. The time scale for significant montmorillonite transformation at repository temperatures in natural sediments is orders of magnitude longer than the period of elevated temperature in a KBS-3 repository /e.g. Velde and Vasseur 1992/.
2. The bentonite material is close to mineralogical equilibrium to start with /e.g. Fritz et al. 1984/.
3. Transformation is limited by low transport capacity, principally regarding potassium /Hökmark et al. 1997/ and silica /Karnland and Birgersson 2006/.
4. All published kinetic models, based both on natural analogues and laboratory experiments indicate that the transformation rate is very slow under repository conditions /e.g. Huang et al. 1993/.

The montmorillonite transformation process can also be quantified by modelling, as exemplified above. Based on the above description, no mineral transformation is expected to be faster than illitization as a result of elevated temperature. Consequently, the maximum temperature effect is modelled by the kinetic expression for illitization proposed by Huang et al. and by use of different but realistic potassium concentrations. Adverse pH conditions could lead to increased dissolution of the montmorillonite and possible mass loss.

Two safety function indicator criteria have been defined. As long as the maximum temperature is below 100°C and the pH of the water in the rock is below 11 the montmorillonite in the buffer is assumed to be stable for the timescale of the repository.

In the reference evolution, alteration is not expected to proceed to a level where it will affect the properties of the buffer. Alteration is therefore treated as a separate scenario.

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 neoformed silica impurities will also be calculated.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

Montmorillonite alteration is one of the most studied processes in clay mineralogy and the above argumentation is supported by numerous peer reviewed articles and conference papers available in the open literature. Those cited above represent only a minor fraction of what is available and the key issues are rather the relevance and relative quality of the peer reviewed material. A literature study with reference to specific KBS-3 conditions, including validation of alteration models was made by SKB /Karnland and Birgersson 2006/ in order to address these issues. This report may be seen as a comprehensive evaluation of the adequacy of references.

Uncertainties

Uncertainties in mechanistic understanding

There is a generally accepted explanation of the diagenetic processes by 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 for 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-Site

Laboratory experiments have shown transformation rates that are faster than predicted by the kinetic models under the following extreme conditions. Consequently, these are not covered by the present models:

- Influence of low water content /Couture 1985/.
- Extreme potassium ion concentration /Lee et al. 2010/
- pH effects:
 - high pH: /Velde and Vasseur 1992, Savage et al. 2002, Gaucher et al. 2004, Karnland et al. 2007, Savage et al. 2010/.
 - Low pH: /Zysset 1992/.

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

Thermodynamic and kinetic data for modelling silica dissolution/precipitation are not readily available 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 constants are determined in laboratory experiments performed over relatively short durations and at higher temperatures and potassium concentrations when compared to the conditions they aim to simulate. The various illitization models currently available show a large variety in constant values and model formulae, which indicates conceptual problems. However, the set of determined constants and formulae generally results in similar long-term predictions /Karnland and Birgersson 2006/.

3.5.10 Iron – bentonite interaction

Overview/general description

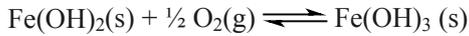
Metallic iron will be present in several places in the repository; the iron insert in the canister, in the supercontainer in the KBS-3H concept and in rock reinforcements. The amount of iron is considerable, especially in the KBS-3H concept. The fact that metallic iron is not thermodynamically stable in the repository ($E^0 < 0$ V) raises the questions: where does it go and what does it do? The answer is complex and implies that it depends on several factors such as the redox potential, the temperature, the pH, solute concentrations and the composition of the buffer. Other less obvious factors may also be important such as the buffer density, temperature gradients, transport rates and microbes.

Standard iron corrosion in the absence of bentonite

The initial step in anaerobic corrosion takes place as follows:



If any oxygen is present, the reaction that follows is:



If carbonate concentrations are sufficiently high, carbonates will precipitate:



If carbonic acid is absent, Fe(OH)_2 will precipitate, which is stable in the absence of oxygen at low temperatures. At higher temperatures ($> 373 \text{ K}$), it will convert to the thermodynamically more favoured magnetite phase. The reaction is also possible at lower temperatures but is then much slower.



This possible build-up of magnetite and other corrosion products can passivate the iron surface and decrease the corrosion rate.

Iron corrosion in the presence of bentonite

The anaerobic corrosion of iron does not seem to be passivated in the same way in bentonite. The corrosion rate seems to be increased by the presence of bentonite. This is possibly due to the cation exchange capacity of the clay minerals which allows them to adsorb iron ions thereby minimising precipitation. In addition, corrosion and/or its products seem to react with the clay minerals creating new non-swelling minerals /Lantenois et al. 2005, Perronnet et al. 2008/.

The most probable scenarios are:

- Formation of ion exchanged iron-montmorillonite.
- Reduction of the iron in the octahedral sheet of the montmorillonite structure, possibly coupled to dehydroxylation (reversible or irreversible).
- Dissolution and/or transformation of the montmorillonite.
- Formation of corrosion products with possible cementation of the buffer.

All scenarios will probably affect the buffer performance to some extent. The rate and degree of destabilisation of the smectite seems to depend on the nature of the smectite (dioctahedral/trioctahedral, counter ion and Fe^{III} - content) /Lantenois 2005/. The effect of iron reduction may have a negative impact on the hydraulic conductivity and the swelling properties. The cation fixation capacity has been observed to increase /Khaled and Stucki 1991/.

Dependencies between process and buffer variables

Table 3-17 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Site.

Boundary conditions

The relevant boundary condition for this process is the presence of iron in the adjacent system components. As long as the canister is intact, the only source of iron is in the construction materials within the repository. In the case of a failed canister, there will be large amounts of iron in close contact with the buffer.

Table 3-17. Direct dependencies between the process “Iron – bentonite interaction” and the defined buffer variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Buffer geometry	Yes, through transport of dissolved species and total buffer mass	Included in mass balance	Yes, for extreme unexpected transformation	Separate scenario
Pore geometry	Yes, through transport of dissolved species and ion equilibrium	Included in model/ expression used	Yes, by definition	Separate scenario
Radiation intensity	No		No	
Temperature	Yes	Neglected, since the reaction will occur late in the repository evolution	No	
Water content	Yes, through transport of dissolved species	Full saturation assumed	Yes, for extreme unexpected transformation	Neglected, importance is minor
Gas content	Yes, through transport of dissolved species	Neglected, since the reaction will occur late in the repository evolution	No	
Hydrovariables (pressure and flows)	Yes, minor through transport of dissolved species	Neglected since the major source of iron is present inside the canister	Yes, for extreme unexpected transformation	Separate scenario
Stress state	No, pressures are too small to be significant		Yes, for extreme unexpected transformation	Separate scenario
Bentonite composition	Yes, through available species in accessory minerals	Neglected, due to small effect compared to other sources	Yes	Precipitation of iron phases can be calculated
Montmorillonite composition	Yes, by definition	Included in model/ expression used	Yes, at extreme unexpected transformation	Separate scenario
Porewater composition	Yes, by definition	Included in model/ expression used	Yes, by definition	Included in model/ expression used
Structural and stray materials	Yes, determines availability of iron	No iron is assumed to be present as stray material in buffer	(No)	

Model studies/ experimental studies

Most of the published results are based on experiments where the kinetic limitations have been reduced in some way. The most common ways to speed things up is to increase the temperature, increase the liquid/solid ratio or to increase the reactive surface area by intimately mixing iron and clay powders. However the experimental results are very sensitive to the conditions and hence the results from the studies are rather scattered /Mosser-Ruck et al. 2010/.

Typical experimental results are the following examples:

- (i) Iron powder mixed with different bentonites in deionised water was heated at 80°C for 45 days. Ion exchange was noticed, and also magnetite and 7 Å phyllosilicate formation /Lantenois et al. 2005/.
- (ii) Carbon steel (coupons and wires) in compacted MX80 bentonite was heated (30 and 50°C) with artificial groundwater for up to 900 days. No transformation of the montmorillonite was observed. Magnetite, hematite and goethite were identified as corrosion products. The results were consistent with sodium to iron ion exchange of the montmorillonite /Carlson et al. 2007/.
- (iii) FoCa7 bentonite was mixed with various ratios of powdered metallic iron in Evian water and heated for 45 days at 80°C. The ratio of clay and iron seems to have an impact on the new phases formed. SiAlFe gels were created, which matured into Fe-rich phyllosilicates (identified as odinite or greenalite) /Perronet et al. 2008/.

Iron bentonite interaction is studied in the Alternative Buffer Materials (ABM) project at Äspö HRL. Eleven different compacted clays are placed in contact with an iron heater at 130°C in three different packages. The experimental time is from two to more than five years. The clays have been selected to give a broad variation in properties, such as smectite content, iron content, counter ion composition and accessory minerals.

Natural analogues/observations in nature

Possible analogues could be naturally occurring native iron (meteoritic or non-meteoritic) or perhaps old archaeological artifacts in contact with bentonites or other clays. However because of the rare nature and the uncertain history of the objects they are probably of limited value. Other natural analogues could be soils in anaerobic environments in rice fields where Fe-rich chlorites or 1:1 minerals have been identified /Favre et al. 2002/.

Time perspective

The process may occur as long as iron is present in the repository.

Handling in the safety assessment in SR-Site

Since there will be very small amounts of iron present in the vicinity of the deposition hole, the process is assumed to be of insignificant importance to the buffer properties as long as the canister is intact.

For the case of a defective canister, alteration of some of the buffer caused by the interaction with metal iron cannot be ruled out based on current knowledge.

Iron-clay interaction was not assumed to change the major properties of the buffer in the SR-Can assessment. This will still be the assumption in SR-Site. However, since there are uncertainties regarding this process a sensitivity discussion will be included in the montmorillonite transformation scenario.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

All references included are peer reviewed scientific publications. General corrosion of iron in an anaerobic environment at the level presented here is rather well known. The probable iron-bentonite interaction scenarios listed are based on those indicated by experiments, both specific to the topic and in montmorillonite transformation in general.

Uncertainties

Uncertainties in mechanistic understanding

There are uncertainties in the mechanistic understanding and the total possible impact from the metallic iron on buffer properties.

Model simplification uncertainties in SR-Site

No quantitative model is available. The possible consequences will be discussed with simple sensitivity studies.

Input data and data uncertainties in SR-Site

Not really applicable in this case.

3.5.11 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 3.4.1 Swelling/mass redistribution). Fractures intersecting the deposition hole mean that rigid swelling

restrictions are not present everywhere, and that localized swelling continues into the fractures until an equilibrium or steady state is reached. This free swelling may lead to separation of individual montmorillonite layers (dispersion) and part of the buffer could be transported away by groundwater.

The maximum free swelling of the bentonite is strongly dependent on the valence and concentration of the ions in the interlayer space. At low groundwater concentrations, the interlayer distance between the individual montmorillonite layers may increase enough to give the clay/water system a sol character, i.e. single or small groups of montmorillonite layers act as individual colloidal particles.

The maximum interlayer distance, when only monovalent ions are present in the solution, may be discussed in terms of the Debye-Hückel screening length, which is inversely proportional to the square root of solution concentration. The same dependence on interlayer separation with solution concentration has been experimentally determined /Norrish 1954a, b/. The forces between parallel montmorillonite layers with only monovalent ions present, can be calculated for an ideal system from DLVO theory /Derjaguin and Landau 1941, Verwey and Overbeek 1948/, in which the entropic repulsive effects from ions and the attractive van der Waals forces are taken into account. In the case that only divalent ions are present in the system, additional attractive forces become significant, which restrict the swelling to relatively short interlayer distances and prevent release of individual colloid particles /Guldbrand et al. 1984, Kjellander et al. 1988/. However, a relatively small content of monovalent ions in a calcium-dominated system may still lead to general colloidal sol formation in deionised water or at very low ion concentrations /Birgersson et al. 2010, Hedström et al. 2011/.

For simple model systems such as charged spheres or parallel extended flat charged surfaces, the concept of a critical coagulation concentration (CCC) is readily defined within the DLVO theory as the salt/electrolyte concentration where the energy barrier for particle-particle association approached zero /e.g. Evans and Wennerström 1999/. At the CCC and higher salt concentrations the attractive van der Waals forces dominate the system and colloidal particles will be held together and not disperse spontaneously. If one considers montmorillonite as extended negatively charged surfaces ordered in parallel, the calculated CCC for a 1:1 salt e.g. NaCl within DLVO theory turns out to be in the range 1–2 M. However, experimentally the transition from sol to attractive gel is observed to take place at much lower concentrations /van Olphen 1963, Le Bell 1978, Hetzel and Doner 1993, Abend and Lagaly 2000, Wold 2003, Lagaly and Ziesmer 2003, Tombács and Szekeres 2004/. This strongly suggests interactions other than face-to-face DLVO forces, in real montmorillonite systems. It has been proposed /van Olphen 1963/ that flocculation of clay could be a result of the interactions between positive charges present on the edges of clay particles and negative charges on the faces of the clay particles. /Missana and Adell 2000/ have shown that the small fraction of the pH-dependent charges on the edge greatly influence the stability behaviour of the clay colloids and that the standard DLVO theory for parallel clay layers is not particularly suitable for predicting the stability, mainly because it is not able to account for this charge contribution. However the concept of a CCC need not be defined within the framework of a particular theory but from observations alone as the concentration where an attractive gel can be formed /e.g. Abend and Lagaly 2000/.

A CCC may be determined for monovalent systems and used as a conservative concentration limit for spontaneous colloid particle release. Governing variables are the concentration and the layer charge of the montmorillonite. Laboratory results have shown that montmorillonite extracted from MX-80 bentonite and ion-exchanged to Na⁺-state has a CCC of around 25 mM in NaCl solution, i.e. an attractive gel is formed /Birgersson et al. 2010/. Two other Na- montmorillonites analyzed with higher layer charge than in MX-80 were found to have lower CCC, in contrast to predictions from DLVO theory for parallel layers /Evans and Wennerström 1999/. For systems with only divalent counterions the CCC concept is not really valid, and the CCC may be considered zero, i.e. no excess ions are needed in order to prevent colloidal sol formation of colloidal particles as demonstrated in (e.g. Ch 4 in /Birgersson et al. 2010/) or from theoretical considerations /Kjellander et al. 1988/. For a mixed system with both mono and divalent counterions one also needs to consider ion equilibrium /Kahn 1958/. Thus one cannot speak in terms of a CCC for Ca²⁺ for Na-montmorillonite as such a value cannot exist. The limiting condition for colloidal sol formation (sol formation) is thereby given by combinations of ion concentrations and monovalent/divalent ion ratios in the clay/water system illustrated in Figure 3-29.

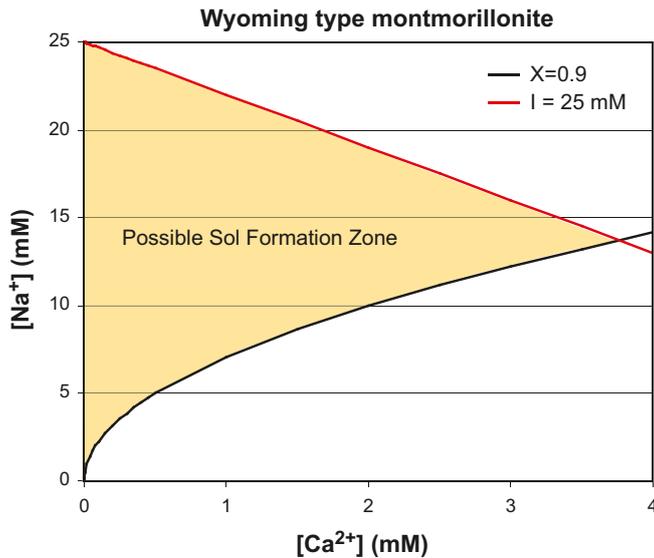


Figure 3-29. Limitations of a possible sol formation zone for Wyoming type montmorillonite in equilibrium with an external Ca/Na-solution and monovalent anions (e.g. Cl⁻). The lower curve ($X=0.9$) represents the experimental finding that when the Ca fraction is 0.9 or higher in the clay no sol is formed irrespective of the ionic strength in the external solution. On the upper curve the ionic strength equals 25 mM, which is the CCC value for Wyoming-type montmorillonite in NaCl solution /Birgersson et al. 2010, 2011/.

The central conditions for possible colloid formation in a repository are consequently the local porewater concentration and the ratio between mono and divalent ions in the montmorillonite at the bentonite/groundwater interface. The governing processes are ion exchange of the original montmorillonite counterions by ions originating from the accessory minerals and from the surrounding groundwater.

Loss of bentonite material may be significantly reduced, or even eventually stopped, by space limitations under mineralogical/chemical conditions which lead to sol formation. Laboratory results have shown that pore sizes smaller than 0.5 microns completely prevent the montmorillonite particles penetrating filters, but pore-sizes of 2 micron or larger do not restrict the loss significantly, as illustrated in Figure 3-30. This figure shows the swelling pressure evolution of a compacted 5 mm thick disc of Na-montmorillonite confined by filters of pore size 2 or 10 μm according to the set-up in Figure 3-31. Behind the filters deionised water is circulated at a pumping rate of 1 mL/min. The drop in swelling pressure seen in Figure 3-30 is caused by montmorillonite loss through the filters. The fact that filters with pore size of 2 μm do not prevent montmorillonite loss is in accordance with measured particle size distributions /Michot et al. 2004, Karnland et al. 2006/. In a repository an auto healing effect may be present as a result of clogging fractures by accessory minerals of different grains sizes.

Based on present knowledge, significant formation of colloids and subsequent buffer mass loss cannot be excluded over the time scale of several glaciations.

Table 3-18 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Site. 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 valence of the groundwater in direct contact with the outermost part of the bentonite buffer and also the cation pool in the bentonite itself.

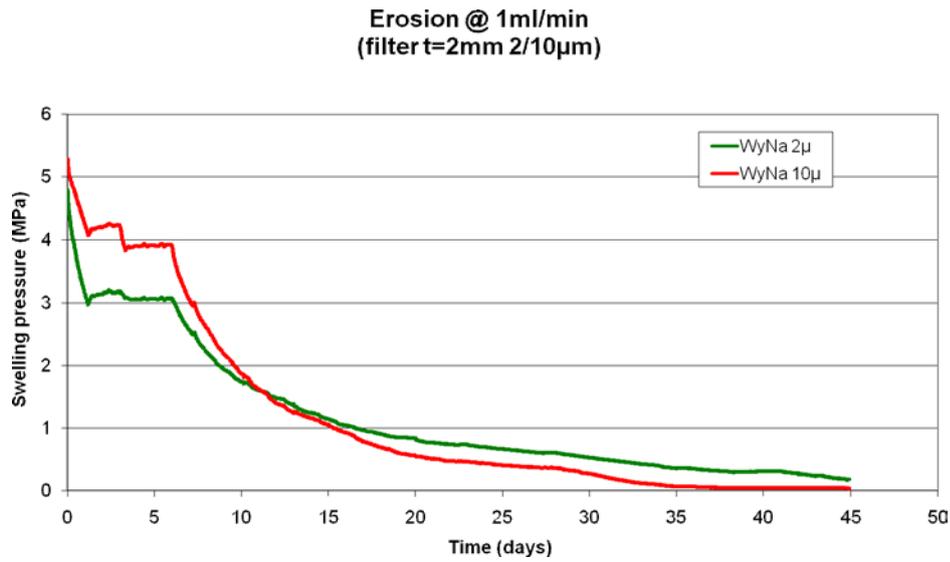


Figure 3-30. Swelling pressure for Wy-Na montmorillonite as a function of time using filter pore sizes of 2 and 10 mm respectively. The drop in swelling pressure is caused by loss of clay through the filters (2 mm thick). /Birgersson et al. 2010, Hedström et al. 2011/.

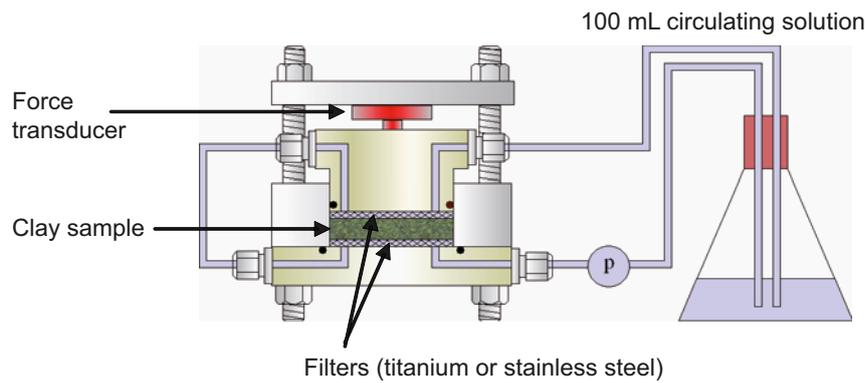


Figure 3-31. Schematic drawing of the swelling pressure test cell /Birgersson et al. 2010/.

Table 3-18. Direct dependencies between the process “Montmorillonite colloid release” and the defined buffer variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Buffer geometry	Yes, the amount of buffer present	Included in modelling	Yes, at extreme process magnitude	Included in modelling
Pore geometry	Yes, governs the dispersing forces	Included in modelling	Yes, by definition	Included in modelling
Radiation intensity	No		No	
Temperature	No, negligible		No	
Water content	Yes, by definition	Full saturation assumed	Yes, by definition	Full saturation assumed
Gas content	Yes, no dispersion possible from unsaturated clay	Full saturation assumed	No	
Hydrovariables (pressure and flows)	Yes, by definition	Included in modelling	Yes, indirect through pore geometry, central impact	Evaluated from modelling results
Stress state	Yes, by definition	Included in modelling	Yes, major impact	Included in modelling
Bentonite composition	Yes, impurities may govern the ion type and concentrations	Included in modelling	Yes, selective loss of the clay component	Included in modelling
Montmorillonite composition	Yes, important variables are magnitude and distribution of layer charge, and type of cations	Included in modelling	Yes, possible through selective formation of colloids	Neglected
Porewater composition	Yes, major importance both with respect to cation type and concentration	Included in modelling	Yes, through pore geometry	Included in modelling
Structural and stray materials	Yes, concrete, especially, may provide calcium ions	Neglected, no concrete assumed in buffer	Yes, minor effects possible through calcium uptake	Neglected

Water flow in the fractures will not affect the stability of the sol phase. 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 tear loose montmorillonite even before the clay formally turns into a sol. The extent of such particle release by flow is dependent on the flow velocity. Without flow the particles will sediment. The treatment of erosion is presented in Section 3.3.4.

Model studies/experimental studies

The principles for swelling of montmorillonite in 1:1 electrolyte solutions have been reported in a large number of publications. The basic theoretical principles are described by the DLVO theory /Derjaguin and Landau 1941, Verwey and Overbeek 1948/. For divalent cations additional attractive correlation forces come in to play which necessitates a theoretical treatment beyond the DLVO theory /Gulbrand et al. 1984, Kjellander and Marčelja 1984, Kjellander et al. 1988/. Interlayer distances were experimentally determined by Norrish /1954a, b/, and several subsequent studies have in principle confirmed these results, e.g. those by /Zhang and Low 1989/. Several laboratory studies have been made in order to determine the critical coagulation concentration for montmorillonite in sodium chloride solutions /van Olphen 1963, Le Bell 1978, Hetzel and Doner 1993, Abend and Lagaly 2000, Wold 2003, Lagaly and Ziesmer 2003, Tombács and Szekeres 2004, Laaksoharju and

Wold 2005, Birgersson et al. 2010/. A large body of work suggests the mechanism for montmorillonite coagulation in NaCl is edge-face interactions /e.g. Lagaly and Ziesmer 2003, Tombács and Szekeres 2004, Birgersson et al. 2010/ although opinions differ concerning the pH range where the edge charges may be positive.

Ion exchange must be considered for mixed mono- and divalent systems. Such systems may be described in terms of a sol formation zone (SFZ) as shown in Figure 3-29. Experiments have established that the upper boundary of the SFZ is significantly lower than predicted by the ionic strength assumption; thus the zone is much smaller than depicted in Figure 3-29 and limited to a very thin region close to the $[\text{Na}^+]$ -axis /Birgersson et al. 2010, 2011/. Thus, in order to prevent colloidal sol formation a much lower ionic strength than 25 mM is needed in mixed Ca/Na montmorillonite systems. The possible colloid release at low ionic strength has further been investigated using swelling pressure cells where the region near the $[\text{Na}^+]$ -axis has been explored by circulating initially pure NaCl solutions contacted with mixed Ca/Na montmorillonite. At low ionic strength, the NaCl solution is close to the equilibrium solution because very little Ca/Na exchange will occur because under such conditions nearly all of the calcium remains in the montmorillonite. The outcome from such experiments /Birgersson et al. 2010/ is shown in Figure 3-32 Swelling pressure evolution of eroding test CaNaErosion02 /Birgersson et al. 2010/. The montmorillonite is of Milos type and the ion population is 50/50 Ca/Na. The circulating solution is 2 mM NaCl at the beginning of the time period displayed. The pumping rate has been lowered by a factor of 4 or 16 compared to the original rate throughout the test period. The effects of changing pumping rate are indicated in the diagram. The points at which the circulating solution has been replaced by a solution of lower concentration are also indicated. Note that cessation of erosion around day 15 occurs spontaneously, without changing pumping rate or circulating solution. At day 57 the solution is changed to deionised water and loss of montmorillonite starts again, which demonstrates the connection between sol formation and ionic strength: erosion can be controlled physicochemically.

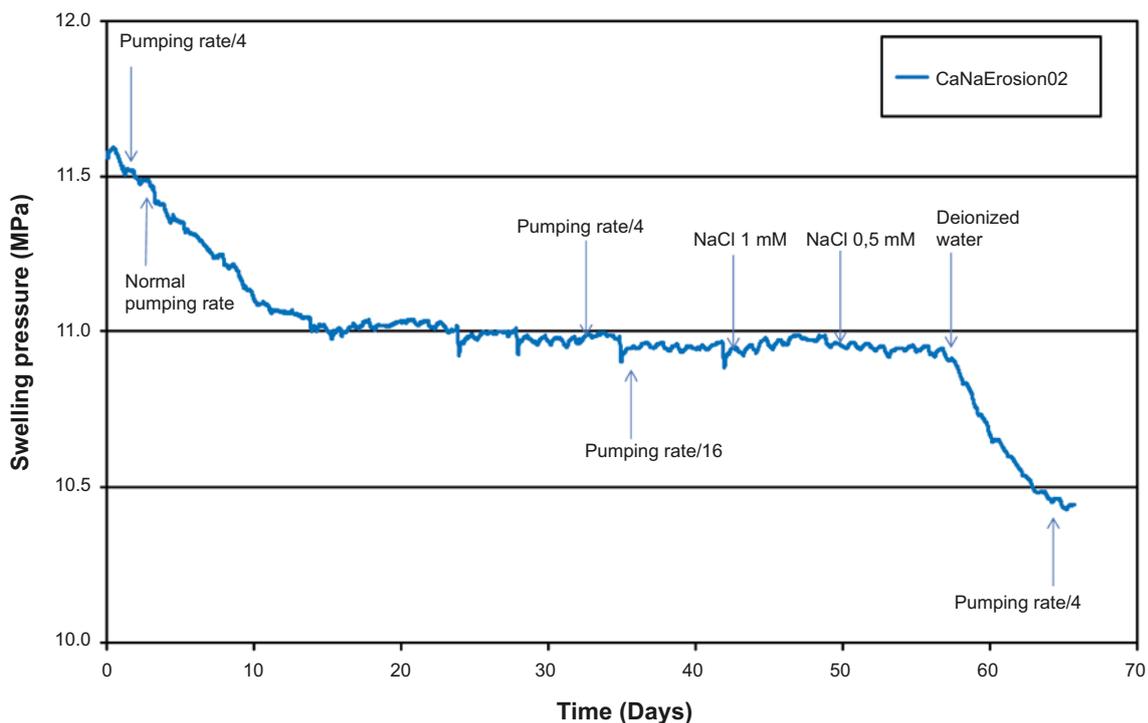


Figure 3-32. Swelling pressure evolution of eroding test CaNaErosion02 /Birgersson et al. 2010/. The montmorillonite is of Milos type and the ion population is 50/50 Ca/Na. The circulating solution is 2 mM NaCl at the beginning of the time period displayed. The pumping rate has been lowered by a factor of 4 or 16 compared to the original rate throughout the test period. The effects of changing pumping rate are indicated in the diagram. The points at which the circulating solution has been replaced by a solution of lower concentration are also indicated. Note that cessation of erosion around day 15 occurs spontaneously, without changing pumping rate or circulating solution. At day 57 the solution is changed to deionised water and loss of montmorillonite starts again, which demonstrates the connection between sol formation and ionic strength: erosion can be controlled physicochemically.

and loss of montmorillonite starts again, which demonstrates the connection between sol formation and ionic strength: erosion can be controlled physicochemically and Table 3-19. Since charge is conserved one may define the concentration where sol formation ceases in terms of positive charge equivalents. This definition also encompasses the scenario where the circulating solution initially contains calcium that will be almost totally exchanged for sodium at equilibrium.

The experimental SFZ shows the behaviour of montmorillonite in thermodynamic equilibrium with an external solute having a given composition of Na⁺ and Ca²⁺ (monovalent/divalent cations). The composition of the glacial Grimsel water /Auqué et al. 2006/ is such that it is below the SFZ, thus montmorillonite in equilibrium with Grimsel water will be calcium-dominated and not form colloidal sols. One key component in understanding the sol formation process and whether the loss of bentonite will be critical is the approach to equilibrium. Modelling attempts within the Bentonite Erosion Project have been carried out, using various counterion compositions in the initial bentonite and various ionic compositions of the seeping groundwater. The evolution of the buffer is then calculated based on diffusion of ions and ion exchange at the buffer/groundwater interface /Neretnieks et al. 2009a, 2009b/. A pessimistic approach has been taken assuming that buffer will be lost as colloidal sol if the Ca²⁺ fraction in the buffer at the interface falls below 0.9 (see SFZ Figure 3-29). The modelling suggests that for some combinations of the initial and boundary conditions, the fraction of Ca²⁺ in the clay may fall below 0.9. Modelling taking the upper limit of the SFZ into consideration has not yet been carried out.

Within the Bentonite Erosion Project the DLVO based force-balance model for spherical colloids /Petsev et al. 1993/ has been adapted to parallel clay layers /Liu et al. 2009, Neretnieks et al. 2009b/ and used to calculate the swelling of Na-montmorillonite into fractures filled with water of low ionic strength (1:1 salt). The force-balance model uses DLVO to describe swelling pressure and Kozeny-Karman-like expression fitted to experiments to describe hydraulic conductivity. The model is adjusted and tested towards free-swelling experiments obtained through magnetic resonance imaging (MRI) /Dvinskikh et al. 2009/. Advective loss of montmorillonite is modelled by combining the force-balance model for swelling with a viscosity model for the repulsive montmorillonite gel and the Darcy equation for two-dimensional flow in a fracture intersecting the deposition hole. The outcome of the modelling for different water velocities in a 1 mm aperture fracture is shown in Table 3-20. The montmorillonite release rate is found to be proportional to the water velocity to the power 0.41 and directly proportional to the aperture.

Table 3-19. Summary of the erosion experiments conducted with Ca/Na-montmorillonite in /Birgersson et al. 2010/. X denotes the charge fraction of calcium in the clay. The column “Observed stability” lists the lowest NaCl concentration for which no (or undetectable) erosion occurred.

Sample	Clay Type	X	Observed stability
CaNaErosion01	Milos	0.5	2 mM
CaNaErosion02	Milos	0.5	0.5 mM
CaNaErosion03	Milos	0.25	1 mM
CaNaErosion04	Milos	0.75	3 mM
CaNaErosion05	Wyoming	0.5	4 mM
CaNaErosion06	Kutch	0.5	1 mM

Table 3-20. Loss of smectite by advective flow /Neretnieks et al. 2009b/.

Water Velocity, m/yr	Smectite release for 1 mm fracture aperture, g/yr	Penetration into the fracture at the centre, m
0.10	11	34.6
0.32	16	18.5
0.95	26	11.5
3.15	43	7.0
31.50	117	2.1
315.00	292	0.5

Natural analogues/observations in nature

In principle, a large number of analyses of Swedish groundwater may serve as natural analogues 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/.

A literature review of bentonite deposits with the objective of finding natural analogues was done as a part of the Bentonite Erosion Project /Puura and Kirsimäe 2010/. However, the conclusion was that relevance to the Bentonite Erosion Project is still questionable because of the uncertainties related to the changes during tens and hundreds of millions of years.

Time perspective

Colloid formation is only relevant at low ion concentrations and likely to be relevant only in conjunction with a glaciation. The effects may be significant only in the long-term perspective.

Handling in the safety assessment SR-Site

Water with cation content higher than 2–4 mM charge equivalents is considered to prevent colloidal sol formation provided that the calcium content in the montmorillonite is above 20%, irrespective of whether the montmorillonite is of Wyoming, Milos or Kutch type. This criterion is also in agreement with reported amounts of calcium salts needed to coagulate initially homoionic Na-montmorillonites /Swartzen-Allen and Matijević 1976, Hetzel and Doner 1994, Lagaly and Ziesmer 2003/. Ion exchange processes during the operation of the repository may alter the counterion content relative to the initial state. However the content of calcium is not expected to fall below 20%. Thus the process of colloidal sol formation can be neglected during normal operating conditions. Present day ground water at both the Forsmark and the Laxemar sites fulfil this condition as does Baltic Sea water. During glacial conditions the cation content may possibly fall below 2–4 mM charge equivalents, and colloidal sol formation can therefore not be excluded.

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. The model is based on the relationship that the montmorillonite loss rate is proportional to the water velocity to the power 0.41 and directly proportional to the aperture as proposed in /Neretnieks et al. 2009b/. The underlying force-balance model in /Neretnieks et al. 2009b, Liu et al. 2009/ is based on DLVO for parallel surfaces and therefore not valid for divalent counterions and does not include edge-face interactions. The model thus assumes that the bentonite consists of only montmorillonite which is converted to a pure Na-form and the buffer porewater 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, erosion is assumed to occur at a rate that is determined by the product of the equivalent flow rate at the deposition hole. This model maximises the loss rate assuming that the mass exchange between the bentonite suspension and the flowing water is driven by diffusion. Correlation effects present for divalent counterions as well as edge-face interactions contribute attractive forces. The omission of these is also considered to be conservative.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

The presence of attractive correlation forces beyond the DLVO theory for systems with divalent counterions is well established in peer reviewed journals, e.g. /Guldbrand et al. 1984, Kjellander and Marčelja 1984, Kjellander et al. 1988/ as well as in advanced textbooks e.g. /Evans and Wennerström 1999/.

Gel-sol transition in sodium montmorillonites around the CCC value for NaCl and other sodium salts has been studied using various methods, such as e.g. visual inspection, turbidity measurements rheological measurements and been reported in peer reviewed journals /Hetzl and Doner 1993, Abend and Lagaly 2000, Lagaly and Ziesmer 2003, Tombács and Szekeres 2004/. /Laaksoharju and Wold 2005/ use visual inspection and their results are in agreement with those in peer reviewed journals. /Birgersson et al. 2010/ (part of the Bentonite Erosion Project) also finds CCC values for NaCl in accordance with published data. Furthermore they stress the importance of ion-equilibrium in mixed Ca/Na systems which lead to the concept of a sol formation zone in Na^+ - Ca^{2+} concentration space. The criterion that sol formation is prevented when the cation content in the groundwater is higher than 2–4 mM charge equivalents and calcium content in the clay is larger than 20% /Birgersson et al. 2010/ is also supported by findings reported in peer reviewed journals /Swartzen-Allen and Matijević 1976, Hetzel and Doner 1994, Lagaly and Ziesmer 2003/.

The handling of colloidal sol formation in SR-Site will be based on the documentation produced in the Bentonite Erosion Project, e.g., /Birgersson et al. 2010, Neretnieks et al. 2009b/. These documents as well as other supporting work have undergone formal internal SKB review. The intention is also to publish relevant parts in peer reviewed journals and two such articles, /Birgersson et al. 2011, Hedström et al. 2011/ regarding the influence of Ca-ions and sol formation at low ionic strength, have been accepted for publication. The derivation of the force-balance model is published in peer reviewed journals /Petsev et al. 1993, Liu et al. 2009/. The development of the MRI technique for studying free swelling of bentonite/montmorillonite has also been published in a peer reviewed journal /Dvinskikh et al. 2009/.

Uncertainties

Uncertainties in mechanistic understanding

Knowledge concerning colloidal sol formation and colloid stability is good concerning the effects of mono- and divalent ions. However, modelling of the correlation effects caused by divalent ions is demanding. The prevention of sol formation at low ionic strength when the calcium content in the montmorillonite is above 20% has been verified experimentally. Detailed understanding of this effect is less well developed and handling edge-face interactions in modelling is unsolved. The force-balance model is based on parallel layers and furthermore only tested versus vertical swelling experiments and for short swelling times, up to 5 weeks. The possible transport of colloids by diffusive and flow transport is less well known. The effects of mechanical erosion of loose gels close to sol forming conditions have not been fully examined. Experiments show that montmorillonite does not penetrate filters with pore-sizes of 0.5 mm. However, it has not been shown that accessory minerals could actually form an effective filter in the fractures. The understanding of the effect pH on colloidal sol formation is incomplete.

Ca/Na ion exchange also influences the swelling properties of montmorillonite / Kjellander et al. 1988, Birgersson et al. 2010, 2011, Hedström et al. 2011/, which means that a more realistic modelling of bentonite swelling into fractures should include ion correlation effects /Guldbrand et al. 1984, Kjellander and Marčelja 1984, Kjellander et al. 1988/ as well as edge-face interactions that cause coagulation at low ionic strength /Lagaly and Ziesmer 2003, Tombács and Szekeres 2004, Birgersson et al. 2010, 2011/.

Model simplification uncertainties for the above handling in SR-Site

The treatment for quantifying montmorillonite loss during glacial conditions in SR-Site is based on the model in /Neretnieks et al. 2009b/. 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 assumption that the force-balance model is conservative for the swelling of Na-montmorillonite. Predicted CCC is claimed to be about 50 mM whereas the underlying DLVO model gives 1–2 M.
2. Assumption of Darcy flow.
3. Disregarding wall friction is assumed to be conservative.

The following could act to decrease the dispersion rate:

1. The change of composition in the diffuse layer is not accounted for.
2. The presence of 20% or more Ca in the clay.
3. A model beyond DLVO for parallel clay layers. Correlation as well as edge-face interactions.
4. Physical hindrance of clay particle dispersion in the fracture.
5. Clogging of pathways by the clay being pressed out into the fracture.
6. Sedimentation of clay particles in fracture.

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

The evolution of groundwater composition, and groundwater flow conditions are the important uncertainties. These will be evaluated in integrated assessment modelling, see further the Interim report of the safety assessment SR-Site. The state of the buffer with respect to monovalent/divalent ion ratio and content of accessory minerals at the time of contact with glacial water of low ionic strength is uncertain. Diffusion coefficients for Ca and Na and their variation with water ratio are also uncertain.

3.5.12 Radiation-induced transformations

Overview/general description

This process covers the direct effect of radiation on the stability of the montmorillonite component of the buffer material. Indirect effects through the radiolysis of porewater are covered in that process (see Section 3.5.13).

Montmorillonite in the buffer can potentially be broken down by γ -radiation. The result is a decrease in the montmorillonite component of the buffer.

In the case of a failed canister, radionuclides sorbed in the buffer could possibly affect the properties by α -radiation.

Dependencies between process and buffer variables

Table 3-21 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Site.

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, see Section 3.1.1.

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 abundance. MX-80 bentonite saturated with weakly brackish water to a density of 2,050 kg/m³ was irradiated for one year with a total radiation dose of $3 \cdot 10^7$ Gy, which is orders of magnitude more than will be the case in the repository. The specimen was confined in a cylinder with one closed end consisting of iron and irradiated with a ⁶⁰Co source, while the other end consisted of a porous steel filter through which a water pressure of 1.5 MPa was imposed /Pusch et al. 1993b/. 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, showed no significant change in the montmorillonite quantity in either of the specimens.

Table 3-21. Direct dependencies between the process “Radiation-induced transformations” and the defined buffer variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Buffer geometry	Total buffer mass available	Dose rates are too low to cause any significant transformations – the process is excluded from SR-Site	No	
Pore geometry	No		No	
Radiation intensity	Yes	Dose rates are too low to cause any significant transformations – the process is excluded from SR-Site	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-Site
Montmorillonite composition	Not detected		(Yes)	Dose rates are too low to cause any significant transformations – the process is excluded from SR-Site
Porewater composition	No		No	
Structural and stray materials	No		No	

The buffer will not be exposed to α - and β -radiation as long as the canister is intact. In the case of a failed canister, radionuclides that migrate out will be sorbed in the buffer and may expose it to a radiation dose.

In the radionuclide calculations for SR 97 /SKB 1999/, 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. In most parts of the buffer, the α -dose will be much less since the α -emitters are strongly sorbed and will stay in the vicinity of the canister. $8 \cdot 10^{15}$ alphas/g corresponds to an absorbed dose of 8 MGy. /Gu et al. 2001/ show that the amorphisation dose for montmorillonite is 30 GGy. Since the total dose received is more than three orders magnitude lower than the amorphisation dose, the impact on the properties of the buffer can be expected to very small.

Natural analogues/observations in nature

No studies of systematic studies of clay mineralogy under the influence of alpha radiation are available.

Time perspective

See Section 3.1.1.

Handling in the safety assessment SR-Site

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.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

/Gu et al. 2001/ is a peer reviewed publication in the open literature. The same reference was also used by ANDRA in /ANDRA 2005/. /Pusch et al. 1993b/ is an old SKB report, but there is no documentation available that would indicate that the conclusions would be invalid.

Uncertainties

There are no uncertainties of relevance to the safety assessment.

3.5.13 Radiolysis of porewater

Overview/general description

Gamma radiation from the fuel that penetrates through the canister can decompose porewater by radiolysis, forming OH radicals, H₂, O₂ 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 wall thickness is, however, sufficient so that the effect of γ -radiolysis on the outside is negligible /Werme 1998/. This process is also described in the Fuel and Canister Process Report /SKB 2010k/.

Dependencies between process and buffer variables

Table 3-22 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Site.

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 summarised in /King et al. 2001/. The results show no effect on the corrosion rate even with higher doses than those expected in the repository.

Natural analogues/observations in nature

Not applicable.

Time perspective

γ radiation is significant during the period approximately 1,000 years following canister installation.

Handling in the safety assessment SR-Site

After water saturation, radiolysis of water near the canister will occur. This will lead to the formation of oxidants and hydrogen. If these radiolysis products are not removed, equilibrium will soon be reached whereby further production of hydrogen and oxidants ceases. If the radiolysis products are removed, however, for example by the diffusion of hydrogen away from the canister or by reaction of the oxidants with copper or other oxidisable species in the system, radiolysis can continue. Calculations of radiolysis outside a canister have been made by /Christensen and Pettersson 1997/. An estimate of the maximum possible amount of oxidised copper can be made if one assumes that

Table 3-22. Direct dependencies between the process “Radiolysis of porewater” and the defined buffer variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Buffer geometry	(Determines the total amount of water in the radiation field)		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-Site	No	
Temperature	No		No	
Water content	Yes, determines the amount of water available	Dose rates are too low to cause any significant radiolysis outside canister – the process is excluded from SR-Site	No	
Gas content	No, but indirectly through water content		No	
Hydrovariables (pressure and flows)	No		No	
Stress state	No		No	
Bentonite composition	No		No	
Montmorillonite composition	No		No	
Porewater composition	Determines the reactions	Dose rates are too low to cause any significant radiolysis outside canister – the process is excluded from SR-Site	Yes	Dose rates are too low to cause any significant radiolysis outside canister – the process is excluded from SR-Site
Structural and stray materials	No		No	

the oxidation of copper will be as efficient as the oxidation of dissolved Fe(II) in Christensen’s calculations. After about 10^{10} s (~ 327 years) the amount of precipitated Fe(III) is 1 mol/dm^3 . Assuming that the oxidants present in a 5 mm water layer surrounding the canister reach and react with the copper surface, the total volume of irradiated porewater for a porosity of 0.44 /SKB 2006c/ will, (for canister dimensions $L = 5.85 \text{ m}$, $D = 1.05 \text{ m}$, and neglecting the details of the lid and bottom designs), be:

$$[4.85 \cdot 10.5 \cdot \pi + 2 \cdot (10.5/2)^2 \cdot \pi] \cdot 0.05 \cdot 0.44 \text{ dm}^3 = 39 \text{ dm}^3$$

This gives a total amount of precipitated Fe(III) of 39 moles and, consequently, 39 moles of corroded copper. For a canister area of $[4.85 \cdot 10.5 \cdot \pi + 2 \cdot (10.5/2)^2 \cdot \pi] \text{ dm}^2$ and a copper density of $8,930 \text{ g/dm}^3$, this gives a corrosion depth of approximately $16 \text{ }\mu\text{m}$. Conversely, the experimental observations of /King et al. 2001/ indicate that the overall effect of radiation on copper corrosion under oxidising conditions will be negligible or even result in a lowering of the corrosion rate.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

The calculations in /Christensen and Pettersson 1997/ are directly applicable to the repository situation. The report has been produced within Studsvik's Quality Assurance System according to ISO 9001, which requires review and approval by two different individuals.

Uncertainties

There are no uncertainties currently identified that are of relevance to the safety assessment.

3.5.14 Microbial processes

Overview/general description

Under certain conditions, microbial processes can result in the formation of gas and sulphide /Pedersen 2002/. Gas formation can give rise to pore pressure and mechanical effects in the bentonite 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 canister integrity. This is mainly due to the fact that sulphide is commonly precipitated with ferrous iron. Therefore, sulphide concentrations do not occur at high concentrations in groundwater and its diffusive transport capacity is very low. In order for the processes described above 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 2001, Pedersen et al. 2008/. 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 the safety assessment /Hallbeck and Pedersen 2008/.

Dependencies between process and buffer variables

Table 3-23 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Site.

Table 3-23. Direct dependencies between the process "Microbial processes" and the defined buffer variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Buffer geometry	No, indirectly through pore geometry		No	
Pore geometry	Yes. Microbial activity decreases exponentially with increasing buffer densities and approach nil at densities above 2,000 kg/m ³	Maximal possible production of sulphide and gas is calculated for all possible pore geometries (densities) and the amounts produced are compared with the amount needed to corrode a copper canister	No	
Radiation intensity	Yes	Lethal effects from the radiation field are not considered	No	

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Temperature	Yes. Microbial activity is positively correlated with temperature and will be higher during the thermal period compared to the ambient temperature period	Maximal possible production of sulphide and gas is calculated for high and low temperatures and the amounts produced are compared with the amount needed to corrode a copper canister	No	
Water content	Yes. Decreasing water availability reduces the diversity and the possibilities for microbial activity. At the same time, increasing water content increase the stress state (swelling pressure)	Maximal possible production of sulphide and gas is calculated for all possible water contents and the amounts produced are compared with the amount needed to corrode a copper canister	No	
Gas content	Yes Microbial activity is possible with hydrogen and methane as sources of energy	Maximal possible production of sulphide is calculated for all possible gas contents and the amounts produced are compared with the amount needed to corrode a copper canister	Yes. Microbial activity may result in the production of carbon dioxide and methane	Only effects on the buffer/canister are considered
Hydrovariables (pressure and flows)	(No)		Yes induced gas pressure induces water flow	Neglected since the effect is very small
Stress state	Yes. Microbial activity decreases exponentially with increasing buffer densities and approach zero at densities above 2,000 kg/m ³	Maximal production of sulphide is calculated for all possible pore geometries and the amounts produced are compared with the amount needed to corrode a copper canister	No	
Bentonite composition	Yes. Organic carbon can be utilised and several types of commercial bentonites contain viable bacteria including thermophilic sulphate reducing bacteria	Microbial activity can be possible. Maximal production of sulphide is calculated for the bentonite in use and the amounts produced are compared with the amount needed to corrode a copper canister	Yes.	Neglected since the effect is very small
Montmorillonite composition	Yes. Iron reducing bacteria can use Fe(III) in smectite as an electron acceptor in their respiration	The risk maximum layer charge change is evaluated for the bentonite used	Yes. Iron reducing bacteria may degrade montmorillonite which will decrease the swelling properties of the bentonite	The risk for illitisation is evaluated for different combinations of bentonite process variables. Discussed in the bentonite transformation scenario
Porewater composition	Yes	Maximal production of sulphide and gas is calculated for all possible porewater compositions and the amounts produced are compared with the amount needed to corrode a copper canister	Yes	Only the indirect effects on the buffer/canister are considered
Structural and stray materials	Yes	No stray materials are assumed to be present within the buffer material	Yes	No stray materials are assumed to be present within the buffer material

Buffer geometry: The overall dimension of the buffer will have no direct impact on the process. An expanding buffer – into fractures or into the tunnel could however affect the pore size and impact the pore geometry.

Pore geometry: The density of the buffer affects the pore size. Pores with sizes smaller than about 200 nm cannot 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 tolerable temperature are lethal. The highest demonstrated temperature for active microbial life is 113°C. /Stetter 1996/.

Water content: Decreasing water availability reduces microbial diversity. Many microbes can compensate for low water content using metabolic, energy consuming processes but some water is needed for active life. A combination of low energy availability and low water content is detrimental to many microbes /Potts 1994/.

Gas content: Hydrogen and methane can be consumed by microbes; a large effect is obtained if oxygen is present. Active microbes can produce gas if organic carbon is available for metabolism. Methanogens generate methane from hydrogen and carbon dioxide. Anaerobic methane oxidation (ANME) has been identified as a crucial microbial process. This process outputs sulphide when methane is oxidised with sulphate in the ANME process. Therefore, methane may imply sulphide production where microbial life is possible in the buffer. As judged from results from Olkiluoto, Finland /Pedersen et al. 2008/, and also from the Äspö hard rock laboratory (HRL), the rate can be high. Similarly, hydrogen from depth and/or corroding iron may result in sulphide via microbial processes. When oxygen is present, methane is oxidised with concomitant reduction of oxygen /Eriksson 2007/.

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.

Bentonite composition: There is a positive correlation between microbial activity and the concentration of organic carbon. Previous investigations and ongoing investigations of materials from the Alternative Buffer Materials project at Äspö show that sulphate reducing bacteria are common in many clays. Several of the alternative materials appear to have thermophilic sulphate reducers that grow much better at temperature above 50°C, than at room temperature. It is obvious that many of the buffer materials come with sulphate reducers of which several withstand high temperatures /Masurat et al. 2010a/.

Montmorillonite composition: Iron-reducing bacteria have been demonstrated to dissolve iron-rich smectite through reduction of structural Fe(III) at room temperature and 1 atmosphere within 14 days under good growth conditions /Kim et al. 2004/. Microbial processes may consequently have an influence on the variable if the montmorillonite is rich in Fe(III).

Porewater composition: There is a positive correlation between microbial activity and the concentration of organic carbon. There is a limited effect on the porewater chemistry if the microbes are metabolically active. Gas and sulphide production can 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. See previous discussion under Bentonite Composition. No stray materials are assumed to be present in the buffer.

Boundary conditions

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) and dissolved gas (sources of energy) between the buffer porewater 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/m³ /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 BCE raised questions about the survival of microbes, and especially SRB, in buffer materials with 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 sulphate-reducing bacteria were mixed with MX-80 bentonite at varying saturated bentonite densities, from 1,500 kg/m³ to 2,000 kg/m³ /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/m³. *D. baculatum* survived the better of the two, remaining culturable for 60 days at 1,500 kg/m³. Although microbial activity diminished rapidly, 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 sulphate 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 of 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 bacterial 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 populations. All of the three spore formers survived at the lower 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 sulphate-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 for 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 $^{35}\text{SO}_4^{2-}$. 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 bentonite densities: 1,500, 1,800 and 2,000 kg/m^3 , corresponding to water activities at the unpressurised condition of 0.999, 0.994, and 0.964, respectively. After incubation, $^{35}\text{S-Ag}_2\text{S}$ 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 saturated bentonite density of 1,500 kg/m^3 , but sulphide production was virtually absent at higher densities. This experiment indicated that SRB probably cannot be active at the canister surface at a repository bentonite density of 2,000 kg/m^3 at full water saturation. 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 at full water saturation using stainless steel oedometers with $^{35}\text{SO}_4^{2-}$ as an oxidised sulphur source for the SRB respiratory processes /Masurat and Pedersen 2003, Masurat et al. 2010b/. 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) (experiment B). 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 homogenisation 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 (experiment G) with filter-sterilised groundwater (0.2 μm) was used as control. Finally, a third bentonite set-up was heat treated at 120°C for 12 h and sterile groundwater added. 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 to the final density of the bentonite, as the highest density had the lowest overall SRB activity (Figure 3-33).

The experiments with sterile groundwater on the one hand, and sterile groundwater and heat treatment of the bentonite on the other, 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 there are two sources of SRB to buffer material; the groundwater and the bentonite itself.

Natural analogues/observations in nature

There is a natural analogue in Dunaorobba, 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.

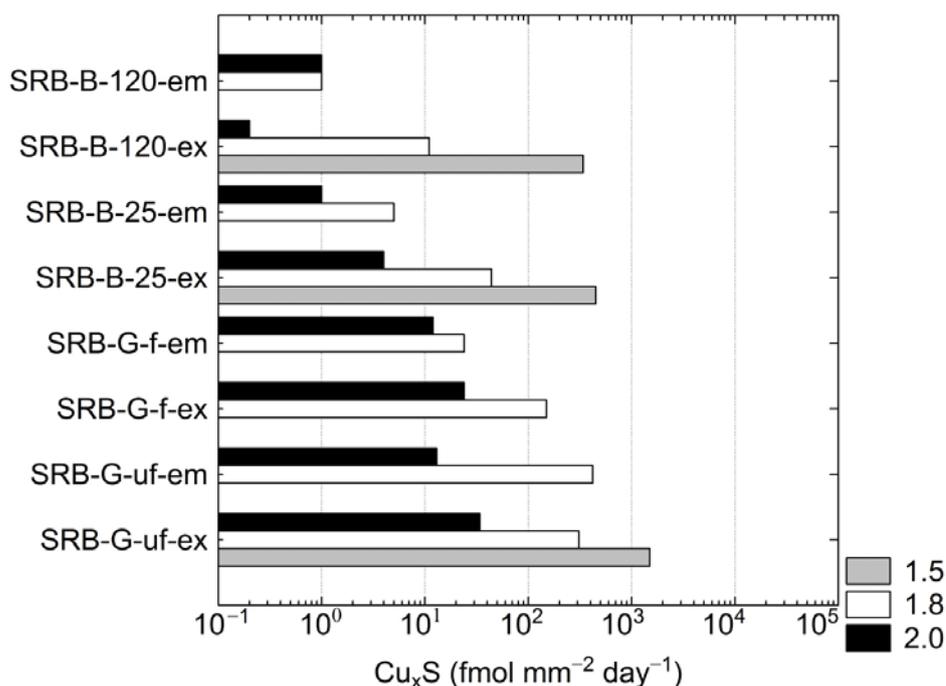


Figure 3-33. Graphic representation of the mean copper sulphide production rates on copper plates that were exposed (ex) and embedded (em) at different saturated bentonite densities (1,500, 1,800 and 2,000 kg m⁻³). The treatments were un-filtered (uf) filtered (f) in experiment G and exposure to 25°C (25) and 12°C (120) during 15 h. See text for details. Figure is from /Masurat et al. 2010b/.

Time perspective

The time perspective concerning survival and activity of microbes in compacted bentonite has been summarised in a conceptual model as follows /confer Figure 3-4 in Pedersen 2002/. 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 all the void volume. This water can be groundwater from the rock or, alternatively, groundwater or process 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.

Swelling of the clay will introduce groundwater microbes into the clay, to a depth that is dependent on the initial slot, on both the rock and the canister side of the bentonite. Additionally, 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. 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. The timing for such sterilisation has not yet been clarified. 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-Site

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 25,000 fmol Cu₂S/mm² a day will

corrode 50 mm depth of a canister in 1 million years /Masurat et al. 2010b/. If the safety limit is set to 25 fmol $\text{Cu}_2\text{S}/\text{mm}^2$ a 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 kg/m^3) under field conditions (Figure 3-33). 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 energy from groundwater, radiation intensity, the water content and the level of heat stress (temperature). For additional information see the process “copper corrosion” in the Fuel and Canister process report /SKB 2010k/.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

All the references in this section are from peer reviewed scientific journals. However, the most recent may be in the progress of being published.

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, energy and sulphide, radiation, water content and heat stress (temperature) 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 defined experimentally.

Formation of biofilms on the canister surface has been suggested to occur. This may be the case during the initial swelling phase. However, those microorganisms will obey the same restrictions as any microbe in other parts of the buffer. The stress from heat and radiation 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 baker's 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, mechanical pressure and other stress factors. The sum of stress factors, radiation, heat, low initial water availability and a high mechanical pressure after saturation of the buffer results in death of the microbes. However, the exact mechanisms for the observed disappearance of viability of microorganisms remain to be clarified. At full water saturation, water activity is fully restored, but a mechanical pressure develops which corresponds to the water activity in the unpressurised clay according to the Kelvin equation.

The low concentration of sulphide observed in many groundwater samples depends on the availability of ferrous iron, if the availability of iron decreases, the aqueous concentration of sulphide will increase, as it does at some depths in Olkiluoto and recently found also in monitored boreholes at Forsmark and Laxemar, where concentrations approach 10–20 mg sulphide/L. pH must be taken into consideration as dissociation of hydrogen sulphide (gas) depends on pH.

Model simplification uncertainties in SR-Site

Not relevant since a quantitative model for microbial processes in the buffer is lacking.

Input data and data uncertainties in SR-Site

Not relevant since a quantitative model for microbial processes in the buffer is lacking.

3.5.15 Cementation

Overview/general description

The term “cementation” has often been used in a broad sense to describe processes, which lead to specific changes in rheology and swelling properties of the buffer material. A number of quite different chemical/mineralogical and mechanical processes could conceivably cause cementation, and these are treated here. The accompanying sections dealing with related processes, i.e. montmorillonite stability, ion exchange, accessory mineral alteration, diffusive transport etc are consequently of most relevance for the cementation process. The main concerns regarding the effects of cementation of the bentonite buffer are increase in hydraulic conductivity reduction of swelling ability and increase of shear strength.

Cementation due to precipitation of minerals and amorphous compounds commonly leads to lower porosity, which in turn usually leads to lower hydraulic conductivity in soil and rock materials. However, the porosity in the bentonite buffer is as high as 43%, and so the low hydraulic conductivity is obviously not due to low porosity but to montmorillonite/water interaction. Consequently, a large reduction in porosity caused by cementation may still lead to an increase in hydraulic conductivity if the montmorillonite/water interaction is reduced or counteracted by cementation.

Bentonite buffer rheology is characterized by low shear strength, i.e. the material deforms at relatively low shear forces. Precipitates may be expected to increase the shear stress and decrease the strain at failure, i.e. the material becomes more brittle. A rock displacement may thereby transmit higher shear stresses to the canister.

The most obvious cause of cementation is precipitation of minerals and amorphous solids in the bentonite. Potential mineral phases include gypsum, or anhydrite at high temperatures, calcite and silica minerals/compounds and iron oxide/hydroxide minerals/compounds. The underlying source of ions may be the molecular structure of the montmorillonite mineral layer, the interlayer space, accessory minerals and the groundwater. The resulting cementation does not necessarily have to appear in the same volume, since released species can be transported in the buffer owing to the prevailing thermal and concentration gradients.

In addition to the mineralogical causes of cementation, there is a (principally) mechanical effect which may be of importance. The swelling pressure at a certain clay density is significantly dependent on the stress history of the bentonite material /Börgesson et al. 1995/. A similar hysteresis may also be apparent in the rheological properties and the mechanical strength in consolidated clay would therefore have higher shear strength than a swollen sample at the same density. Such a purely mechanical cause of rheological changes is expected to have a limited and relatively small effect on buffer performance. At present, SKB is running laboratory tests in order to quantify and better describe such mechanically-induced rheological changes /Dueck 2010/.

The mineralogical processes that lead to cementation may take place at relatively low temperatures, but all experimental data indicate that the processes are only of importance at relatively high temperatures, in response to temperature gradients or after relatively large temperature changes.

Dependencies between process and buffer variables

Table 3-24 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Site.

Boundary conditions

The boundary conditions for the cementation process are the porewater composition, groundwater composition, temperature in different parts of the buffer and the buffer composition.

Model studies/experimental studies

The principal mineralogical processes that may cause cementation are treated separately in the descriptions of underlying processes; mainly Montmorillonite Transformation (Section 3.5.9),

Table 3-24. Direct dependencies between the process “Cementation” and the defined buffer variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Buffer geometry	No		No	
Pore geometry	Yes, through ionic equilibria	See Sections 3.5.6 and 3.5.9, Alteration of impurities and montmorillonite transformation	Yes, main effect	See Section 3.5.6, Alteration of impurities
Radiation intensity	No		No	
Temperature	Yes, major impact	See Sections 3.5.6 and 3.5.9, Alteration of impurities and montmorillonite transformation	Yes, minor effects through changes in thermal conductivity.	Neglected unless modeling shows significant amounts of precipitation
Water content	Yes, Major impact	See Section 3.5.6, Alteration of impurities	Yes, through changes in porosity	See Section 3.5.6, Alteration of impurities
Gas content	Yes, through concentration	See Section 3.5.6, Alteration of impurities	No	
Hydrovariables (pressure and flows)	Yes, through transport of species	See Section 3.5.6, Alteration of impurities	Yes, indirect through pore geometry, central impact	See Sections 3.5.6, 3.5.5 and 3.5.9, Alteration of impurities, sorption and montmorillonite transformation
Stress state	Yes, through ionic equilibria	See Section 3.5.6, Alteration of impurities	Yes, major possible impact by changed rheological properties	See Section 3.5.6, Alteration of impurities
Bentonite composition	Yes, accessory minerals are of major importance	See Section 3.5.6, Alteration of impurities	Yes, by definition in case of precipitation	See Sections 3.5.6 and 3.5.9, Alteration of impurities and montmorillonite transformation
Montmorillonite composition	Yes, through mineral composition and ionic equilibria with charge compensating ions	See Sections 3.5.6, 3.5.5 and 3.5.9, Alteration of impurities, sorption and montmorillonite transformation	Yes, by definition if the underlying process is montmorillonite alteration	See Sections 3.5.5 and 3.5.9, sorption and montmorillonite transformation
Porewater composition	Yes, by definition	See Sections 3.5.6, 3.5.5 and 3.5.9, Alteration of impurities, sorption and montmorillonite transformation	Yes, by definition in case of precipitation	See Sections 3.5.6, 3.5.5 and 3.5.9, Alteration of impurities, sorption and montmorillonite transformation
Structural and stray materials	Yes, especially the concrete and iron	See Sections 3.5.6, 3.5.5, and 3.5.9, Alteration of impurities, sorption and montmorillonite transformation	No	

Alteration of Impurities (see Section 3.5.6), and Sorption (Section 3.5.5). In general, there is extensive knowledge concerning precipitation in soil material and a vast number of publications with regard to natural systems, experimental work and modelling. There are also a number of publications dealing more specifically with cementation in radioactive waste repositories and several are related to SKB projects e.g. /Pusch 1977/, /Pusch et al. 1998/. The CEA/SKB field test at high temperatures (170°C) relative to KBS-3 conditions, which were performed in the Stripa mine, showed extensive precipitation of especially anhydrite but also of silica compounds in the warmest part. The ductility of the innermost centimetre was completely lost and the hydraulic conductivity dramatically increased /Pusch et al. 1993/. Material from the one year LOT S1 test, performed at a maximum temperature of 90°C at the Äspö HRL, did not show any increase in shear strength or in hydraulic conductivity /Karnland et al. 2000/. Material from the LOT A2 test, exposed to a maximum temperature of 130°C for 6 years, had slightly altered rheological properties in the form of reduced strain at failure, but no changes in hydraulic conductivity were found /Karnland et al. 2009/.

Minor mineralogical changes were found in the warm sections in this material; calcium sulphate, in particular, was redistributed and precipitated in the form of anhydrite in the warm sections. No clear correlation was found, however, between the calcium sulphate content and reduced strain. In subsequent laboratory experiments, it was found that a short heating pulse also produced similar changes in the strain at failure. SKB is presently running two laboratory projects concerning cementation in order to quantify the cementation effects of short-term heating, and to identify the mineralogical changes in the LOT A2 parcel in detail. /Arthur and Zhou 2005/ have performed geochemical modelling and concluded that the total extent of mineral mass transfer, represented by spatial and temporal variations in porosity, may be small in a KBS-3 repository throughout the non-isothermal period. Assessing the effects of such changes on buffer performance is problematic, however, because it is unclear how mineralogical changes affect the physical, mechanical and rheological properties of these materials. Further relevant geochemical modelling is presented in the section on Alteration of Impurities 3.5.6.

Natural analogues/observations in nature

There is a vast literature on soil cementation due to mineral precipitation, and it concerns a variety of mineralogical alterations. The challenge is therefore to discriminate processes relevant for repository conditions and to determine the prevailing geological conditions under which the cementation took place; attempts have been made by several groups, e.g. /Pusch and Madsen 1995, Metcalfe and Moore 1998, Pellegrini et al. 1999, Henry et al. 2007/. Cementation effects as a consequence of illitization have been studied by, among others, /Hower et al. 1976, Boles and Franks 1979/.

Time perspective

Cementation is expected to take place mainly during the water saturation phase and within the non-isothermal period. The effects may, at least to some extent, remain during the whole life-time of the repository.

Handling in the safety assessment SR-Site

The mineralogical evolution in the buffer is presently being modelled, and cementation effects will be judged based on the extent of precipitation. Presently, the process is neglected based on the modelling performed previously and experimental results for rheology.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

The modelling part is discussed under Section Alteration of Impurities. The experimental part is published in peer review journals or in SKB internally reviewed reports.

Uncertainties

Uncertainties in mechanistic understanding

The role of bentonite pore structure and the handling of pore space in geochemical modelling are subject to debate. There is a general problem of how to assess changes in mineralogy on buffer performance, because it is not clear how all possible changes affect the physical, mechanical and rheological properties of the bentonite buffer.

Model simplification uncertainties for the above handling in SR-Site

See Section 3.5.6 (Alteration of impurities) concerning the geochemical modelling.

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

See Section 3.5.6 (Alteration of impurities) concerning the geochemical modelling.

3.6 Radionuclide transport processes

3.6.1 Speciation of radionuclides

Overview/general description

This process discusses the speciation of radionuclides in the aqueous phase. Speciation of radionuclides is of importance for sorption and diffusion processes in the buffer. These processes depend on the aqueous radionuclide species that are kinetically and thermodynamically stable under the conditions of interest at the boundary of the buffer, i.e. inside the canister and also on the chemical conditions in the buffer.

Dependencies between process and buffer variables

Table 3-25 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Site.

Boundary conditions

The boundary conditions for the process are the source term from the canister/fuel, i.e. the speciation inside the canister.

Table 3-25. Direct dependencies between the process “Speciation of radionuclides” and the defined buffer variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Buffer geometry	No		No	
Pore geometry	No		No	
Radiation intensity	(The effect from radiolysis in the buffer will be small)		No	
Temperature	Yes. Chemical reactions are temperature dependent	The uncertainty with respect to temperature is considered. However, the temperature range in the repository is expected to be narrow	No	
Water content	No, but indirectly, because porewater composition changes with water content		No	
Gas content	No, but indirectly through porewater composition		No	
Hydrovariables (pressure and flows)	No		No	
Stress state	No		No	
Bentonite composition	Indirectly through porewater composition		No	
Montmorillonite composition	Indirectly through porewater composition		(Sorbed radionuclides will change the smectite composition, but the effect is limited)	
Porewater composition	Yes. Direct dependence	Used in calculation	Yes	Results from calculations
Structural and stray materials	Indirectly through porewater composition		No	

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, such as PHREEQC or EQ3/6 together with a self-consistent thermodynamic database.

Time perspective

This process is relevant for the whole assessment period, but only if there is a canister failure.

Natural analogues/observations in nature

Natural analogues are usually studied for water rock interactions – not for the water phase alone.

Handling in the safety assessment SR-Site

The solubility and speciation of radionuclides is calculated and used as a source term for the modelling of release from a defective canister (See /SKB 2010k/). This is done for a wide range 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-Site are selected based on experiments done under relevant conditions or from thermodynamic sorption models; see Sections 3.5.5 and 3.5.7. The consistency of the predicted speciation with the speciation calculated in the source term will be checked.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

See Sections 3.5.5 and 3.5.7 and Fuel and Canister Process Report (Speciation of radionuclides) /SKB 2010k/.

Uncertainties

Uncertainties in mechanistic understanding

See processes Sections 3.5.5 and 3.5.7.

Model simplification uncertainties in SR-Site

See processes Sections 3.5.5 and 3.5.7.

Input data and data uncertainties in SR-Site

See processes Sections 3.5.5 and 3.5.7. There may also be uncertainties in thermodynamic data. This is discussed in Sections 3.5.5 and 3.5.7.

3.6.2 Transport of radionuclides in the 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 retarding the transport of most radionuclides,
- speciation, will determine the form (including oxidation state) in which the radioelements exist and therefore also its maximum solubility, as well as how the radioelements are sorbed and transported (sorption can thus be viewed as a part of the speciation),
- colloid transport, could enhance the transport of radionuclides,
- radioactive decay will determine how much of the radionuclide inventory will eventually leave the buffer.

All these have been discussed above among the processes occurring in the buffer, or, in the case of decay, under fuel processes.

Dependencies between process and buffer variables

Table 3-26 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Site.

Boundary conditions

The inner boundary for this process is the concentration of radionuclides within a defective canister. The outer boundary is the fractures in the wall of the deposition hole or the deposition tunnel.

Model studies/experimental studies

Not done for relevant conditions. However, the individual processes are studied; see for example Sections 3.5.3 and 3.5.5.

Table 3-26. Direct dependencies between the process “Transport of radionuclides in the water phase” and the defined buffer variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Buffer geometry	Yes. Gives the volumes and geometries available for transport	Geometry is included in RN-transport calculations	No	
Pore geometry	Yes. Determines diffusivity.	Included in data	No	
Radiation intensity	No		No	
Temperature	Yes, transport and chemical processes are generally temperature dependent	Neglected. RN-transport occurs after thermal pulse. The temperature range in the repository will be narrow	No	
Water content	Yes.	Radionuclide transport is assumed to take place when the buffer is saturated	No	
Gas content	Yes.	Radionuclide transport is assumed to take place when the buffer is saturated	No	
Hydrovariables (pressure and flows)	Yes. Determines the exchange with groundwater	Near field flow is considered in calculations	No	
Stress state	No		No	
Bentonite composition	Yes. Determines sorption and transport properties	Included in data See 3.5.3 and 3.5.5	No	
Montmorillonite composition	Yes. Determines sorption and transport properties	Included in data See 3.5.3 and 3.5.5	Yes. By cation exchange	Neglected since effect from radionuclides is small
Porewater composition	Yes. Determines sorption/speciation	Included in data See 3.5.3 and 3.5.5	Yes. Contamination.	Output from RN-calculations
Structural and stray materials	Indirectly through porewater composition	–	No	

Natural analogues/observations in nature

By definition, this process covers the integrated treatment of radionuclide transport in the near field and it is therefore difficult to find applicable natural analogues. Natural analogues could however be used to study the individual processes, e.g. sorption or solubility.

Time perspective

The process is active at all timescales after canister failure.

Handling in the safety assessment SR-Site

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/ and model summary report /SKB 2010n/ 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 Section 3.5.2.
- Diffusion is treated with element-specific diffusivities and porosities (considering specific oxidation states), see Section 3.5.3.
- Sorption is treated with linear sorption coefficients (K_d) for all elements (considering speciation as well as bentonite and porewater composition), see Section 3.5.5.
- Colloid transport is neglected in the buffer, provided the buffer completely envelops the canister and has a dry density of at least $1,000 \text{ kg/m}^3$, i.e. a clay density of at least $1,650 \text{ kg/m}^3$, see Section 3.5.4.
- 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.

In SR-Can, a simplified, analytic model /Hedin 2002/ was 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. It may be possible to use this model for comparison in SR-Site as well.

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 mass 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 radionuclides 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.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

The two models used for radionuclide transport in the near field /Romero et al. 1999/ and /Hedin 2002/ has been verified against each other. /Hedin 2002/ is a peer reviewed publication in a scientific journal.

Uncertainties

Uncertainties in mechanistic understanding

This process is an integration of several other processes all of which have uncertainties (see above).

Model simplification uncertainties in SR-Site

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 in SR-Site

The data uncertainties for the transport parameters in the buffer are presented in Sections 3.5.3 and 3.5.5. All input data to the radionuclide transport calculations will be handled in the SR-Site data report.

3.6.3 Transport of radionuclides in a gas phase

Overview/general description

A pulse of hydrogen gas can be released from a defective canister see Section 3.3.3. 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. Theoretically, I-129 could also be present as elemental iodine, but the amount will be negligible.

Dependencies between process and buffer variables

Table 3-27 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Site.

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 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.

Table 3-27. Direct dependencies between the process “Transport of radionuclides in the gas phase” and the defined buffer variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Buffer geometry	Yes. The buffer volume determines the transport	See 3.3.3	No	
Pore geometry	No. Only for dissolved gases. Indirectly through stress state		No	
Radiation intensity	No		No	
Temperature	Yes, but the thermal phase will be over before high enough gas pressures can be reached	Neglected	No	
Water content	Yes.	The process is assumed to occur only when the buffer is saturated	No	
Gas content	Yes.	The process is assumed to occur only when the buffer is saturated	Yes	Output from transport estimate
Hydrovariables (pressure and flows)	Yes. The gas pressure will be dependent on the hydrostatic pressure	The pressure build up determines the time for gaseous releases	No	
Stress state	Yes. The opening pressure is dependent on the swelling pressure	The pressure build up determines the time for gaseous releases	No	
Bentonite composition	Indirectly via stress state		No	
Montmorillonite composition	Indirectly via stress state		No	
Porewater composition	Yes and also indirectly via stress state that affects solubility/speciation of gases, especially CO ₂	Pessimistically neglected	No	
Structural and stray materials	No		No	

Handling in the safety assessment SR-Site

Radionuclide transport in a gas phase is treated as a separate case in SR-Site. The handling is based on the experiment by /Harrington and Horseman 2003/ presented in Section 3.3.3. 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, a 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 radionuclides that can be transported in a gas phase are C-14 and Rn-222. Since its half-life is of C-14 is 5,568 years, neither the buffer nor the geosphere is expected to significantly delay the transport to the biosphere. Isotope dilution in a gas phase is not considered. Rn-222 has a very short half-life, but is always present inside the canister. Hence, delay in the geosphere could affect the releases, but is pessimistically neglected in SR-Site.

The pathway may either stay open as long as there is a gas production in the canister or open and close as the buffer reseals leading to repeated pulses of gas (see Section 3.3.3). In the first case, the gas is expected to be released at the same rate as it is produced by corrosion after the breakthrough pulse. The second case will lead to repeated pulses of about equal magnitude.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

See Section 3.3.3.

Uncertainties

Uncertainties in mechanistic understanding

The mechanisms for gas release through bentonite are still not fully understood, see Section 3.3.3. Theoretically, I-129 could also be present in a gas phase as elemental iodine, but the amount will be negligible. Some metals and metalloids form volatile methylated and/or permethylated species, whether these could appear in the fuel at low temperature has not been discussed.

Model simplification uncertainties in SR-Site

The handling of the gas transport pathway in SR-Site is based on a few experiments only. The values for opening and steady-state pressures have been selected from these experiments.

Input data and data uncertainties in SR-Site

As mentioned above, the values for gas opening and steady-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. For the time being, this fraction is pessimistically assumed to be 100%. For Rn-222, it is probably fair to assume that all of the inventory will be in the gas phase.

4 Processes in the tunnel backfill

4.1 Thermal processes

4.1.1 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 thermal evolution within the backfill is determined by the canister power, the canister spacing and the rock thermal properties while the thermal processes conditions in the deposition holes are unimportant.

The heat conductivity of the repository host rock is in the range of 2.0–4.0 W/(mK) /Back et al. 2007, Sundberg et al. 2008/. The backfill conductivity is usually set at 1.5 W/(mK) /Börgesson and Hernelind 2000/, but may be lower depending on the degree of saturation. 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 4-1). 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.

Dependencies between process and tunnel backfill variables

Table 4-1 summarises how the process influences and is influenced by all backfill variables and how these effects are treated in SR-Site.

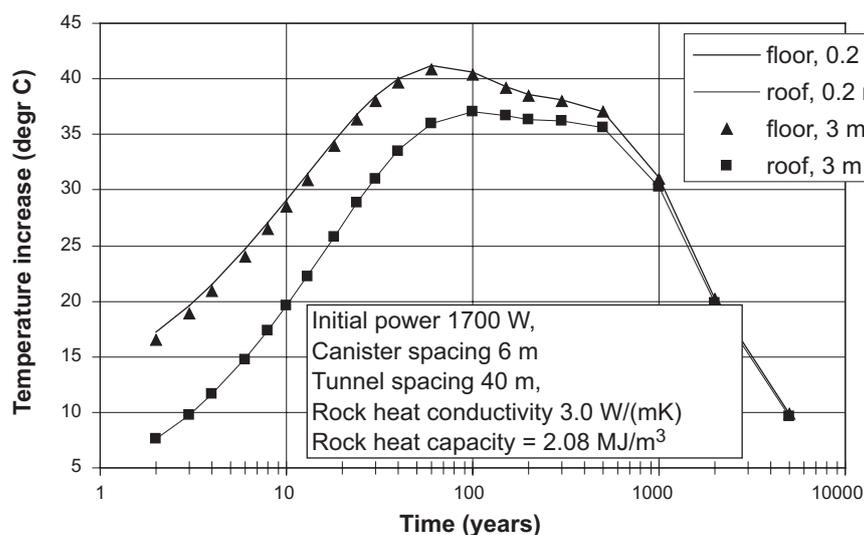


Figure 4-1. Temperatures in tunnel floor and tunnel roof for two positions: 0.2 m and 3 m, respectively, from the axis of the nearest canister. Temperatures are calculated with an analytical solution given by /Claesson and Probert 1996/ without regard to the properties of the backfill.

Table 4-1. Direct dependencies between the process “Heat transport” and the defined tunnel backfill variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable			
	Influence present? (Yes/No)	Description	Handling of influence (How/Why not)	Influence present? (Yes/No)	Description	Handling of influence (How/Why not)
Backfill geometry	Yes		Ignored. The volume occupied by the backfill is sufficiently small that geometry variations are without importance	No, but indirectly via temperature		
Backfill pore geometry	Yes		Neglected, since the thermal expansion of the solid phase will affect the void ratio very insignificantly	No, but indirectly via temperature (and thermal strain)		
Temperature	Yes		Conservatively ignored	Yes		Ignored, since general near-field temperature models confirm that temperatures and temperature gradients within backfill are small.
Water content	Yes		Insignificant in comparison to effects of other processes	No		
Gas content	No, but indirectly through water content			No		
Hydrovariables (pressure and flows)	No			No, but indirectly via temperature		
Stress state	No			No, but indirectly via temperature (and thermal strain)		
Backfill materials – composition and content	Yes		Backfill thermal conductivity given as input data	No		
Backfill porewater composition	No			No		
Structural and stray materials	Yes.		Ignored since the amounts are too small to have any impact	No		

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 are 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, meaning that the backfill temperature will be controlled by the temperature of the surrounding rock, irrespective of geometry variations.

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.

Water content: Conductivity-saturation relations of the type that apply for the buffer are in principle valid also for the backfill, i.e. there is a significant dependence on the water content. Backfill thermal conductivity variations are however not important to the thermal evolution of the near-field, cf. /Kristensson and Hökmark 2007 Hökmark et al. 2009/.

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 porewater pressure and initiate some convective flow.

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 metres below the tunnel floor, and the transport of heat from the near field 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, Hökmark et al. 2009/ and numerically /Thunvik and Braester 1991, 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-Site

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 4.1.2. For these conditions, the backfill temperature can be taken to be equal to that of the host rock. See further the SR-Site Geosphere process report /SKB 2010i/ for the treatment of rock temperatures for these conditions.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

Because of the small thermal gradients and the relatively low temperatures in the backfill there is no specific handling of the heat transport process. The gradient and temperature statements are supported by results obtained using calculation schemes described in /Claesson and Probert 1996/. While that particular report is not peer or factual reviewed, the calculation scheme has been repeatedly applied in peer reviewed papers /Hökmark and Claesson 2005/, and in reports that have undergone (/Hökmark and Fälth 2003/) or will undergo (/Hökmark et al. 2009/) a documented factual and quality review.

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 in SR-Site

Not relevant since the process is not modelled.

Input data and data uncertainties in SR-Site

Not relevant since the process is not modelled.

4.1.2 Freezing

Overview/general description

The overview and general description of the corresponding buffer process, Section 3.2.2, are also valid for the backfill. Since also the backfill material exerts a swelling pressure, freezing (ice formation) is expected to occur at a temperature lower than 0°C.

However, because backfill materials might have a lower content of swelling mineral (montmorillonite), it is crucial to empirically verify that the swelling pressure dependence on temperature still follows the thermodynamic description as described by /Birgersson et al. 2008/.

The swelling pressure of the backfill can be significantly lower than that in the buffer, and it cannot be excluded that it will be frozen in certain time intervals during periods of permafrost. Furthermore, the backfill is extended vertically in ramp and shafts and therefore parts of it will experience temperatures lower than those at repository level. Freezing of the backfill is not a problem per se, as the process has been demonstrated to be reversible. However, it could be imagined that freezing occurs in the backfill in a position closer to surface level while the rock surrounding the repository is frozen. This could lead to increasing pressures in the repository as liquid water is “trapped” in a frozen rock matrix. Such a scenario can only occur, however, when the temperature at repository level is below 0°C and maximum pressure increase can be estimated to 26 MPa /Birgersson et al. 2010/. Note that this is a hydrostatic pressure and will not be harmful to the canisters.

Dependencies between process and tunnel backfill variables

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

Boundary conditions

If the backfill freezes, the water in the surrounding rock will be in ice form. This means that the availability of extra water during ice-lens formation within the backfill probably is very limited.

The effect of freezing on the interaction with the buffer is not clear. There may be a competition for water.

Model studies/experimental studies

A study of the pressure response due to temperature changes of the IBECO-RWC-BF material has been conducted /Birgersson et al. 2010/. The results show a behaviour very similar to what have been measured for the SR-site reference buffer materials (see Section 3.2.2), i.e. a drop in swelling pressure at temperatures below 0°C and no pressure peaks around 0°C has been observed.

Natural analogues/observations in nature

No studies have been conducted. However, knowledge can probably be achieved by studying permafrost areas.

Table 4-2. Direct dependencies between the process “Freezing” and the defined tunnel backfill variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Backfill geometry	Yes, if extended to regions with very low temperatures	Neglected, since only local freezing is discussed	Yes, geometry could change through expansion	Neglected, since no lasting effect on the geometry is expected
Backfill pore geometry	Yes	Yes, see Section 3.2.2	Yes	Included in assessment discussion
Temperature	Yes	Included in assessment discussion	No	
Water content	Yes, via freezing point and transport capacity	Full saturation is assumed when freezing may occur.	Yes, If freezing takes place redistribution of water	Included in assessment discussion
Gas content	(Yes)	1)	No	
Hydrovariables (pressure and flows)	Yes, freezing involves water transport	Included in assessment discussion	Yes	Included in assessment discussion
Stress state	Yes, Influences the freezing point to a small degree	Neglected since effect is small	Yes. Swelling pressure affected also before ice formation	Included in assessment discussion
Backfill materials – composition and content	Yes, via the specific surface area and types of counter ions in montmorillonite	Included in assessment discussion	No	
Backfill porewater composition	Yes, influences the freezing point	Neglected, assessment is based on dilute water	No	
Structural and stray materials	No		No	

1) A gas content would affect the process but the backfill will be completely saturated when freezing

Time perspective

The process of freezing is relevant during the entire repository lifetime.

Handling in the safety assessment SR-Site

The current backfill will have a swelling pressure of ~3 MPa, using the description in Section 3.2.2 the freezing point of the backfill would be around -2°C .

As it has been demonstrated to be reversible, the process of freezing of the backfill is neglected.

Handling of variables influencing the process: The temperature evolution is estimated in /SKB 2010h/.

Handling of uncertainties in SR-Site

Uncertainties in mechanistic understanding

The freezing of soils is a well known process. The description of swelling pressure response due to temperature changes is based on robust, fundamental thermodynamic arguments.

Model simplification uncertainties for the above handling in SR-Site

The reproducibility of the pressure response due to freezing is good. The process can be well described with the equations presented in this section.

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

The bentonite freezing point is strongly dependent on density. If a significant loss of material occurs, e.g. due to chemical erosion, a corresponding change in the freezing behaviour is expected.

Adequacy of references supporting the suggested handling in the safety assessment SR-site

The supporting references /Birgersson et al. 2008/ and /Birgersson et al. 2010/ are a peer reviewed article and a reviewed report according the SR-Site quality system that are available in the open literature. In addition, these particular studies are aimed directly at dealing with the freezing process in swelling clays.

4.2 Hydraulic processes

4.2.1 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 sub-processes are identical to those of the buffer (Section 3.3.1) and will not be reproduced in this discussion.

There are some differences in behaviour and parameter importance between the buffer and the backfill that 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, may be more important for the water saturation process (Boyle's law) of the backfill than the buffer if the backfill is composed of clay with lower smectite content like IBECO-RWC-BF. 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 smectite rich bentonite, the suction potential appears to be sufficiently high for this to occur and full water saturation is achieved without

any external water pressure. IBECO-RWC-BF has lower suction, which means that a pressurised air volume may remain if the air cannot seep out. Due to compression of the air, a large part of the volume will disappear when full water pressure has developed, but the 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 room 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. The rate of diffusion in the backfill is partly 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.

Dependencies between process and tunnel backfill variables

Table 4-3 summarises how the process influences and is influenced by all backfill variables and how these effects are treated in SR-Site. The table illustrates the complexity of this process since all variable influence the process and the process influence all variables but two.

A wide range of materials as backfill candidates has been investigated. They are exemplified by Friedland clay representing the lowest quality (a smectite rich mixed layer clay) and MX-80 representing the highest quality (a high grade Na-bentonite). New tests on IBECO-RWC-BF are recently published /Johannesson et al. 2010/

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. The retention curve is influenced by the temperature (see the buffer).

Influence of water and gas content: See the buffer; Section 3.3.1.

The hydro-variables expressed as suction (negative porewater pressure) in an unsaturated backfill is strongly affected by the water content (retention curve) and the backfill composition. The retention curve of MX-80, IBECO-RWC-BF, Asha and Friedland clay are shown in Figure 4-2 /Johannesson et al. 2010/. It is dependent on several factors as described for the buffer.

The backfill geometry is of course affecting the wetting since the hydraulic gradient depends on 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 the water saturation process 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 pellets filling between the rock and the backfill blocks cannot withstand a high water pressure there will be piping and the water may flow in channels mainly along the rock surface and fill up the voids between the separate pellets. The most likely scenario is that water successively fills the pellets-filled slot and when it reaches the tunnel plug it will not continue past the plug since the plug will be built to resist high water pressure. Instead, water will continue to fill up the pellets-filled slot until all the large voids between the pellets in the entire tunnel are filled with water. There will, of course, be a parallel water uptake and swelling of the backfill blocks in contact with the pellets but if the inflow is not very low it is likely that the entire pellets-filled slot will be water filled before the blocks have swelled and sealed a part of the tunnel. This process is also treated in Section 4.2.4.

Interaction with the buffer: See Section 3.3.1.

Table 4-3. Direct dependencies between the process “Water uptake and transport under unsaturated conditions” and the defined backfill variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence? (How/Why not)	Influence present? (Yes/No) Description	Handling of influence? (How/Why not)
Temperature	Yes, through water viscosity and temperature gradient	Included in the models	Yes, wetting and drying affects thermal conductivity	Neglected since the effects are small in the backfill
Water content	Yes, decisive for the retention curve	Initial water content is given as input data in saturation calculation. The degree of saturation and the void ratio, which determines the water content, are variables in the model.	Yes, changes the water content	Degree of saturation and void ratio are calculated
Gas content	Yes, included in the degree of saturation	Initial gas content is given as input data in saturation calculation. The degree of saturation and the void ratio, which determines the water content, are variables in the model.	Yes, changes the gas content	Degree of saturation and void ratio are calculated
Hydro-variables (pressure and flows)	Yes, main variables in the saturation process	Included variables in the saturation calculation	Yes, changes the hydrovariables	Included variables in the saturation calculation
Backfill geometry	Yes, mainly through distance to wet rock	Given as input data in saturation calculation	Yes. Influencing through the swelling of blocks	See Section 4.3.1
Backfill pore geometry	Yes, the pore geometry influences the water and vapour transport rate.	Included in material data	Yes, through the degree of water saturation that together with the void ratio determines the pore geometry	Degree of saturation and void ratio are calculated
Stress state	Yes, influences the retention curve.	Included variables in the saturation calculation	Yes, changes the swelling pressure	The pressure and suction are calculated
Backfill materials – composition and content	Yes, influenced through the retention curve and other properties	Given as input data in saturation calculation	No, unless via mineral conversion	Not relevant for saturation period
Backfill porewater composition	Yes, influences the hydraulic properties	Included through input data in the saturation calculation	Yes, the composition of the wetting water will influence the backfill porewater composition by definition. Also through ion transport in a temperature gradient	See Section 4.4.4
Structural and stray materials	Insignificant	Excluded	No	

Model studies/experimental studies

A preliminary material model containing unsaturated water flow has been derived (see /Börgesson and Hernelind 1999/) and is being further developed. The models were originally developed for buffer material and can also be used for the 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 process 3.3.1. The model does not include the processes that handle air (except for B2 described above), which can influence the saturation process in the backfill if it consists of Friedland type of clay.

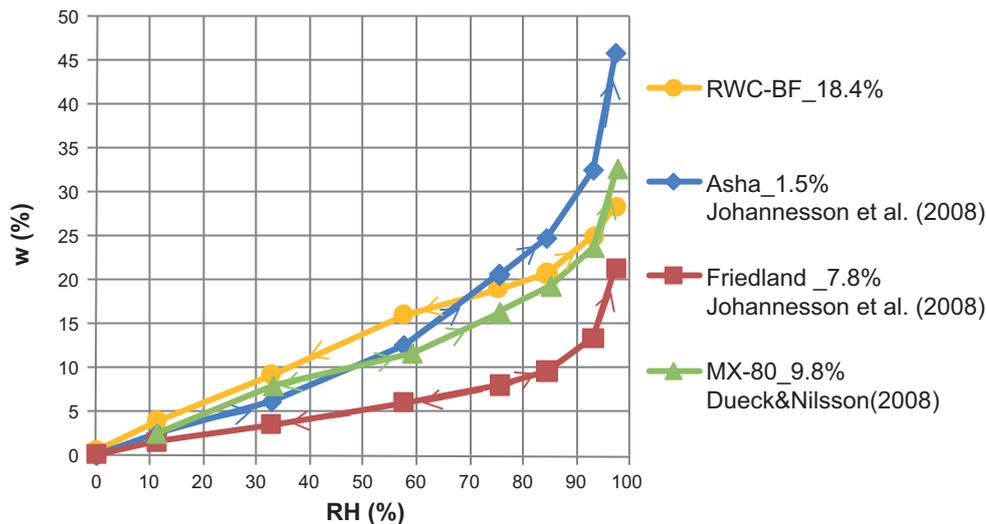


Figure 4-2. Specific retention curve for the RWC-BF material obtained at 25°C shown together with previous results for Asha and Friedland at 25°C and MX-80 at 20°C. The labels show material and initial water content (%). The arrows show the moisture paths /Johannesson et al. 2010/.

The model has been both calibrated and partially verified by laboratory experiments as shown in Section 3.3.1.

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. However, these tests are made with in situ compacted 30/70 mixtures of bentonite and crushed rock and are thus not relevant for the current backfill design. The full-scale tests of deposition holes with canister and buffer are more relevant for studying the behaviour of backfill with high grade bentonite especially the upper part of the deposition holes.

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 SRCan /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 have been done. These calculations will be updated for the new backfill concept /Åkesson et al. 2010a/.

The conclusions drawn from the calculations made for SR-Can are provided below.

The time to complete saturation varies from a few years with 1 m between fractures to more than 150 years with 24 m between the fractures.

Examples of results from the calculations with Friedland clay as backfill are shown in Figure 4-3. However, the calculations assume a homogeneous backfill with a rather low dry density (1,590 kg/m³) and will be updated.

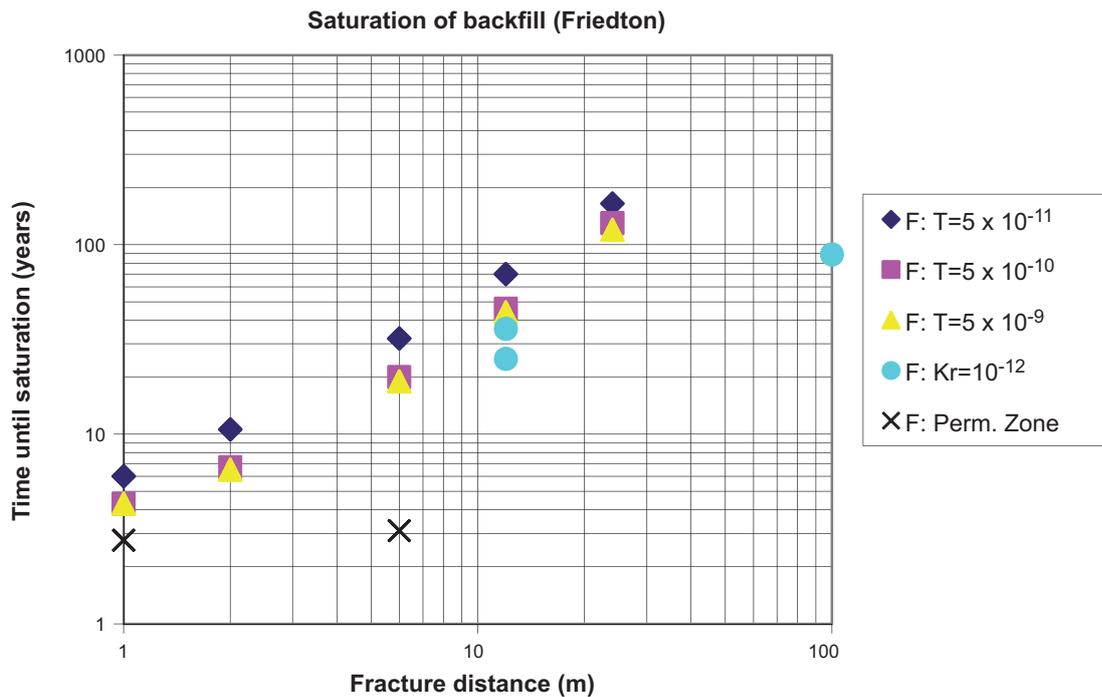


Figure 4-3. Summary of results from calculations regarding Friedland clay (Friedton) backfill with $K=0.7 \cdot 10^{-11}$ m/s in water saturated state. Influence of time until saturation as a function of the fracture distance at different fracture transmissivities T , rock matrix hydraulic conductivity ($K_r=10^{-13}$ m/s in all calculations except two). The influence of a highly permeable zone between the backfill and rock (or extensive piping) is also shown. /Börgesson et al. 2006/

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 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 is thus hindered by the backfill and not by the fracture.

Another conclusion is that the effect of piping and water filling of the pellets-filled slot can be very strong on the rate of wetting since the slot will function as a filter on the rock surface at least in the beginning of the wetting phase.

Natural analogues/observations in nature

Wetting of bentonite in nature has not been studied and can probably not contribute to the knowledge. Manmade bentonite seals are made in completely different ways (mixtures with low density). Natural bentonites have unknown histories

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 in the rock are wet, saturation may be reached within 10 years for a backfill of Friedland clay with low density. If there are no fractures, all water has to go via the rock matrix, which may take several hundred 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-Site

As mentioned above, the initial THM evolution covering the saturation phase of the backfill was 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. However, they are updated in order to take into account the new backfill concept.

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 /Börgesson and Hernelind 1999/. The old calculations have been updated regarding the influence of the backfill. /Börgesson et al. 2006/. 2D rotational symmetric and 2D plane models have been used.
2. Influence of the rock conditions on the wetting phase of the backfill in the deposition tunnels for three different backfill types /Börgesson et al. 2006/. 2D rotational symmetric and 2D plane models have been used.
3. Influence of having entrapped air on the wetting phase of the backfill in the deposition tunnels. These calculations have been done with Code Bright with a material model that includes the air phase. 2D rotational symmetry /Börgesson et al. 2006/.

In addition to this, examples of complete interaction between buffer and backfill with a 3D model have been done /Börgesson and Hernelind 2009/.

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 to some extent control the wetting. Typical timescales range from less than ten to several hundred years.

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

The swelling of the backfill and the bentonite seal following the disintegration of the plug will be analysed with mechanical axis-symmetric 2D Abaqus models. The issue of penetration of bentonite into the central area will also be studied.

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.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

The codes used for modelling the initial THM evolution of the backfill are mainly Abaqus and Code Bright. Abaqus is one of the world's leading general finite element codes that undergoes documented quality controls and has been used in numerous applications reported in peer reviewed articles. The material models used for modelling of unsaturated backfill materials have been assessed in several international projects (see the buffer).

Code Bright is a university code that has been especially designed for THM modelling of unsaturated soils. It has recently been officially available and the code and the material models are steadily updated and assessed in peer reviewed articles.

The main reference for modelling of the wetting scenarios /Börgesson et al. 2006/ is a SKB Technical Report that has not undergone a documented factual- and quality review. However, these calculations will be updated considering the new reference design and the results reported in a general THM modelling report that will undergo a documented factual- and quality review /Åkesson et al. 2010a/. This report will also include modelling of the disintegration phase of the plug.

The main report for the geotechnical properties of IBECO-RWC-BF backfill is /Johannesson et al. 2010/. This report will undergo a documented factual- and quality review.

Uncertainties

The basic hydraulic properties of the backfill materials are rather well known. The main uncertainties of these properties concern the influence of piping and early wetting of the pellets-filled slot.

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. See also Section 4.2.4 (Piping/erosion).

Model simplification uncertainties in SR-Site

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 may not be as good in the backfill as in the buffer. These processes are dealt with in Section 4.2.4 (Piping/erosion) and Section 4.3.1 (Swelling/mass redistribution).

Input data and data uncertainties in SR-Site

The greatest uncertainty/variability concerns the hydraulic conditions in the near-field rock and the hydraulic interaction between the rock and the backfill. The data needed for the modelling are discussed in /Åkesson et al. 2010b/

4.2.2 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 porewater 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 corresponding 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 Section 3.5.8).

The hydraulic conductivity of Friedland clay, as an example, in non-saline water after complete saturation is approximately $2.0 \cdot 10^{-12}$ m/s at the dry density $1,700 \text{ kg/m}^3$ ($2,070 \text{ kg/m}^3$ 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%.

In order to prevent the deposition tunnels from being conductive pathways that influence the water movement 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 on 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 > 100 kPa to ensure a good contact with the rock wall /Gunnarsson et al. 2004/. See also the Design Premises Report /SKB 2009c/.

Dependencies between process and tunnel backfill variables

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

Table 4-4. Direct dependencies between the process “Water transport under saturated conditions” and the defined tunnel backfill variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
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-Site because the thermal pulse will be over when any significant amount of radionuclides may have entered the backfill	No	
Water content	Influenced via density (pore geometry)	Determines the hydraulic conductivity, which is included in the model.	Yes, during swelling since water flow into the voids makes the backfill swell if it can.	Included in the mechanical model
Gas content	Insignificantly (dissolved gases)	Excluded since it would reduce hydraulic conductivity	(Advective transport of dissolved gases)	See Section 4.4.1
Hydrovariables (pressure and flows)	Yes, main variables	Included in the flow model	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, mainly by the flow path	Given as input data.	Yes, during swelling since water flow into the voids makes the buffer swell if there is space available.	Included in the mechanical model
Backfill pore geometry	Yes, determines the hydraulic conductivity	The pore geometry can be affected by a mineral transformation or a change in porewater composition. The effects are discussed in Sections 4.4.7 and 4.4.6	Yes, during swelling since water flow into the voids makes the buffer swell if there is space available.	Included in the mechanical model
Stress state	Yes. If the effective stress on the backfill deviates from the swelling pressure the bentonite will change volume and water will flow into or out from it.	Included in the mechanical model.	Yes	Included in the mechanical model
Backfill materials – composition and content	Yes, determines the hydraulic conductivity (see text)	Included in the model	No	
Backfill porewater composition	Yes, determines the hydraulic conductivity (see text)	Included in the model	Yes	Replacement of porewater is discussed in Section 4.4.4
Structural and stray materials	Insignificant		No	

A wide range of materials as backfill candidates has been investigated. They are exemplified by Friedland clay, representing the lowest quality (a smectite rich mixed layer clay), and MX-80, representing the highest quality (a high grade Na-bentonite).

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 porewater and the temperature.

For Friedland clay, the influence of density and salt concentration in the porewater has been investigated /Pusch 2001, Johannesson and Börjesson 2002/.

For MX-80: see the buffer Section 3.3.2.

For other backfill candidates the measured hydraulic conductivity as a function of the dry density is shown in Figure 4-4 /Johannesson and Nilsson 2006/. Data for IBECO RWC-BF is available in /Johannesson et al. 2010/ and shown in Figure 4-5.

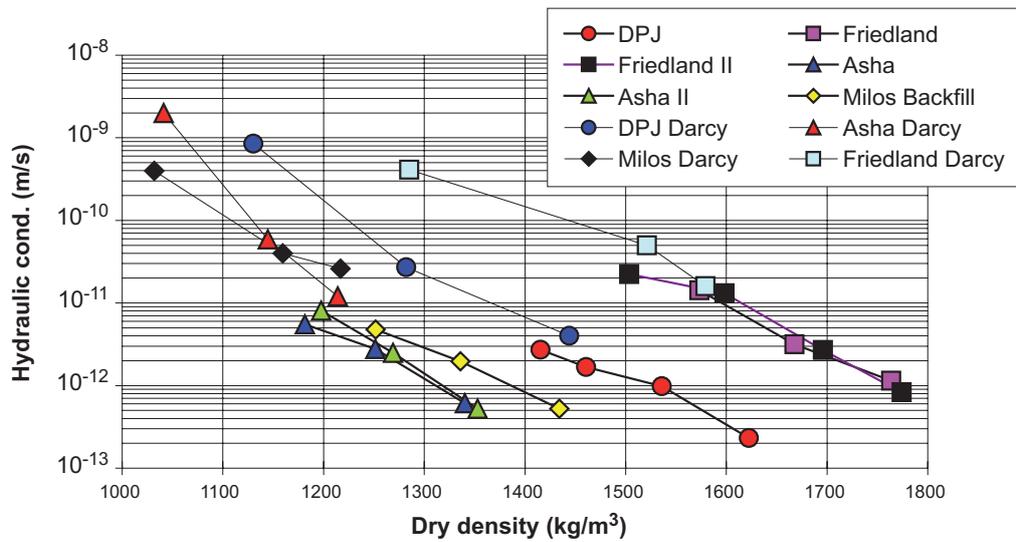


Figure 4-4. Measured hydraulic conductivity as a function of dry density of different backfill candidates. Measurements have been done by applying a hydraulic gradient (termed Darcy) or are evaluated from oedometer tests /Johannesson and Nilsson 2006/.

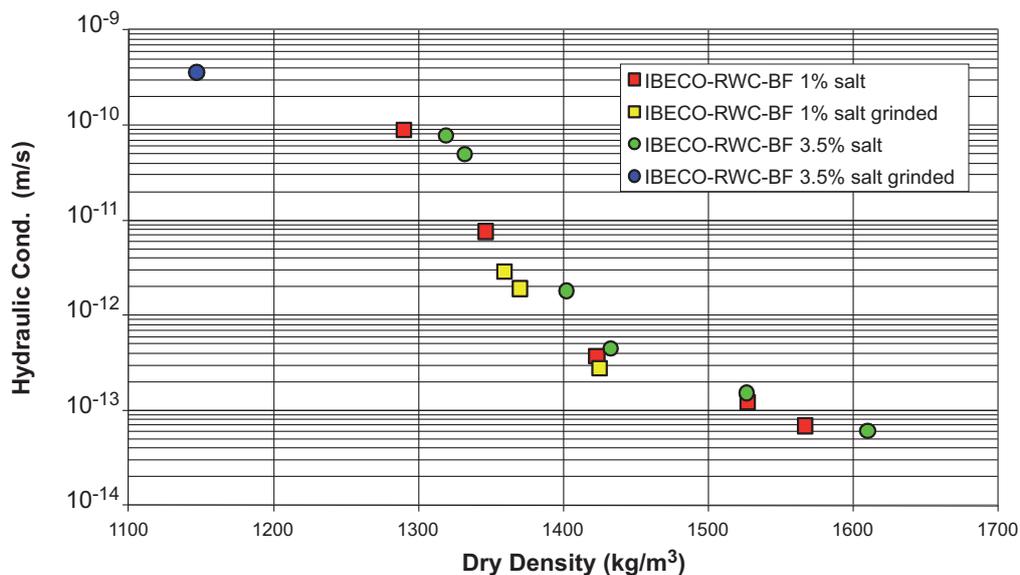


Figure 4-5. The hydraulic conductivity as function of the dry density for the reference backfill material (IBECO-RWC-BF) /Johannesson et al. 2010/

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 60°C entails an approximate increase in conductivity by a factor of 2.

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 in laboratory scale in the form of permeability tests (see references in Figures 4-4 and 4-5) and in full scale in the Backfill and Plug Test /Gunnarsson et al. 2001/. However, the results from this latter test are of limited value since the backfill was composed of a mixture of 30/70 bentonite/crushed rock.

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 has been investigated. The results relevant for IBECO-RWC-BF are reported in /Johannesson et al. 2010/.

Natural analogues/observations in nature

No studies of water flow in natural backfill-like formations have been undertaken for several reasons; the main being that the measured values from the laboratory 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 could be considered because they may yield valuable information on long term behaviour.

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-Site

The change from in situ compacted mixtures to blocks of natural swelling clay or bentonite as backfill material has resulted in a very low hydraulic conductivity that fulfils the conductivity demands with high margins. The base case with an unaltered backfill that has not lost any material

will thus not be investigated in any special way. However, sensitivity analyses are performed where the objective is to identify the parameter space where changes in conductivity result in 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 4.4.6.

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 4.3.1.

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 4.3.1. Consideration will also be given to pressure transients induced by earthquakes.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

The main references of results of hydraulic conductivity measurements on the backfill materials and the influence of different factors are /Johannesson et al. 2010/ and /Karnland et al. 2006/. These reports will undergo a documented factual- and quality review.

Uncertainties

Uncertainties in mechanistic understanding

The uncertainties in mechanistic understanding are the same as those for the buffer (Section 3.3.2).

Model simplification uncertainty in SR-Site

The model used is empirical, connecting hydraulic conductivity to temperature, density and ionic strength of the porewater. 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 of the backfill and before final closure. However, the created channels are expected to heal when the water flow is stopped and the backfill composition is designed for this. This ability of the backfill to be healed is checked in the tests in the project “Backfilling and closure of the deep repository”.

Another uncertainty is the inhomogeneity of the backfill in macro scale. The concerns are if blocks that are friction-fit together may experience incomplete swelling and homogenisation of the slots, if they can close and heal pipes that have eroded and if the pellets filled parts will be sufficiently compressed during homogenisation and swelling of the blocks. All these uncertainties are investigated in the project: “Backfilling and closure of the deep repository” /Gunnarsson et al. 2004/. The most recent findings from the project is presented in /Keto et al. 2009/.

Input data and data uncertainty in SR-Site

Input data for the study of hydraulic conductivity are primarily the empirical relationships between hydraulic conductivity and density, temperature and porewater composition. In SR-Site, this is handled by sensitivity studies with different hydraulic conductivities in the tunnels.

4.2.3 Gas transport/dissolution

Overview/general description

Transport of gas in the backfill can occur in two phases of the repository evolution.

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 groundwater in the rock may contain dissolved gas. This was discussed in Section 4.2.1.

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. The backfill could then act as a sink and decrease the gas pressure in the near field of the repository. 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-Site.

Dependencies between process and tunnel backfill variables

Table 4-5 summarises how the process influences and is influenced by all backfill variables and how these effects are treated in SR-Site.

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. The buffer and the tunnel plugs are also geometrical boundaries for this process, but they will be of limited importance, since the transport capacity for gas in the rock will be much higher.

Model studies/experimental studies

The influence of trapped air on the saturation time was 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 was 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 porewater and then diffuse away, the diffusion rate has a great importance for the saturation process. If the porewater 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 analogues/observations in nature

Not applicable for the backfill.

Table 4-5. Direct dependencies between the process “Gas transport/dissolution” and the defined tunnel backfill variables and a short note on the handling in SR-Site.

Variable	Variable influence on process?		Process influence on variable?	
	Influence present? (Yes/No) Description	Handling of influence? (How/Why not)	Influence present? (Yes/No) Description	Handling of influence? (How/Why not)
Temperature	Yes, but insignificant, since the temperature in the backfill will remain low	Neglected	Yes, wetting and drying affects thermal conductivity	Neglected since the effects are small in the backfill
Water content	Yes, the water content decides the gas content and is decisive for the retention curve	See 4.2.1	Yes, affects the water content	See 4.2.1
Gas content	Yes by definition	See 4.2.1	Yes, changes the gas content	See 4.2.1
Hydro-variables (pressure and flows)	Yes, main variables in the saturation process	See 4.2.1	Yes, changes the hydrovariables	See 4.2.1
Backfill geometry	Yes, mainly through distance to wet rock	See 4.2.1	Yes. Influencing through the swelling of blocks	See 4.2.1
Backfill pore geometry	Yes, the pore geometry influences the water and vapour transport rate.	See 4.2.1	Yes, through the degree of water saturation that together with the void ratio determines the pore geometry	See 4.2.1
Stress state	Yes, influences the retention curve.	See 4.2.1	Yes, affects the swelling pressure	See 4.2.1
Backfill materials – composition and content	No, but indirectly through water content		No	
Backfill porewater composition	No		Yes, gases can dissolve in the porewater	Neglected, of no concern
Structural and stray materials	Insignificant	Excluded	No	

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 of the rock is low the preliminary conclusion was that trapped air is not a very significant factor unless the rock is almost saturated with gas.

Handling in the safety assessment SR-Site

The influence of trapped air on the saturation time of the backfill is investigated in SR-Site. The process involving trapped air is only relevant during the saturation phase (see Section 4.2.1).

The backfill could potentially act as a sink for the escape of corrosion gas from the canister. However, the beneficial effect is rather limited /Wikramaratna 1993/ and the process is not considered in SR-Site. The desaturation of the backfill from gas transport is expected to be very minor with the same reasoning as for the buffer (see Section 3.3.3).

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

The influence of trapped air in the backfill will be investigated in the integrated THM-report which will be formally reviewed. Gas release through the backfill is pessimistically neglected in SR-Site.

Uncertainties

The parameter values for the modelling 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.

4.2.4 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 localised to fractures that carry more water than the backfill can absorb, there will be a build-up of water pressure in the fracture and therefore an increase in the hydraulic gradient across the backfill. The backfill close to the rock surface initially consists of pellets with low density. 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 will be piping, formation of a channel and a continuing water flow, water filling of the space between the pellets and erosion. The processes are described in Section 3.3.4 (buffer). The knowledge of this process and its consequences for the backfill seems to be sufficient today (/Sandén and Börgesson 2010, Sandén et al. 2008/) but research is ongoing.

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 self-heal. 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.

Dependences between process and tunnel backfill variables

Table 4-6 summarises how the process influences and is influenced by all backfill variables and how these effects are treated in SR-Site.

Boundary conditions

The piping and erosion that are treated here mainly take place in the pellets-filled part between the clay blocks and the rock.

Model studies/experimental studies

The processes are studied in the following projects:

- KBS-3H project,
- Baclo project,
- Buffer installation project.

The process and these projects are described in Section 3.3.4.

Natural analogues/observations in nature

Piping and erosion may occur in natural deposits but has so far not been studied. The very special circumstances with the high water pressure at repository depth make such observations doubtful.

Time perspective

The piping and erosion only takes place before complete saturation and homogenisation. The high swelling pressure of the clay will ultimately always seal the piping channels since the swelling ability of the reference backfill (IBECO RWC-BF) is high.

Table 4-6. Direct dependences between the process “Piping/erosion” and the defined tunnel backfill variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Temperature	No		No	
Water content	No, but 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	Yes. 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. Erosion will change the final water content.	The effect of piping on the saturation rate of the backfill will speed up the saturation. The change in final water content due to erosion is modelled (see Sections 3.3.1 and 3.3.4)
Gas content	No, but the degree of saturation and the porewater pressure in the backfill will indirectly influence 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)	Yes, basic variables	The hydraulic gradient, the water flow and the duration are included in the estimate of piping and erosion	Yes	The pipes are assumed to seal when the hydraulic gradients are restored. An “after piping” hydraulic conductivity based on the loss of mass is estimated
Backfill geometry	The distance to the plug influences the water pressure gradient	The effect of piping is evaluated with a simplified mass-balance approach	Yes, through lost backfill material	Amount of lost backfill material is estimated
Backfill pore geometry	Yes, by influence of void size distribution in the pellets slot and Indirectly through the stress state	Included in the mass balance estimations	Indirect through stress state	
Stress state	Yes, determines if piping occurs	Included in the consequence estimation	Yes	An “after piping” swelling pressure distribution is estimated
Backfill materials – composition and content	Yes, the backfill and montmorillonite composition affects variables that are important	Included in the consequence estimation made indirectly through stress state	No	
Backfill porewater composition	The salinity of the water affects many variables that are important for disposition 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-Site

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. See also Section 3.3.4.

In SR-Site, the magnitude of this process is estimated and the results will be used as an input for analyses of the water transport under saturated conditions (Section 4.2.2).

Model: The maximum consequences of this process is estimated by model calculations. This will be based on the experiences from the reported studies and the model according to Equation 3-13 in Section 3.3.4.

Time periods: The process is only relevant during saturation before the water pressure gradient is taken by the plug. 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 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 localised loss of backfill density, which is calculated for different cases.

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

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

Equation 3-13 in Section 3.3.4 will be used to estimate the effect of internal erosion of bentonite in a deposition tunnel. The main reference for this model is /Sandén et al. 2008/.

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 and it is assumed that the process cannot be stopped by the backfill itself until the hydraulic gradient has been reduced. The tests performed for the backfill project have yielded better understanding. The end plug needs to be rather tight in order to stop the erosion.

4.3 Mechanical processes

4.3.1 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 3.4.1 for the buffer. The same basic process description is valid for the backfill.

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.

Some erosion with loss of backfill material is expected to take place during the installation and saturation phase. The channels and possible holes caused by the lost backfill are expected to be healed by swelling and homogenisation of the backfill. Additional measurements and calculations in order to verify this are ongoing (see Section 4.2.4).

Dependencies between process and tunnel backfill variables

Table 4-7 summarises how the process influences and is influenced by all backfill variables and how these effects are treated in SR-Site.

A wide range of materials as backfill candidates has been investigated. They are exemplified by Friedland clay representing the lowest quality (a smectite rich mixed layer clay) and MX-80 representing the highest quality (a high grade Na-bentonite). New tests on IBECO RWC-BF (Milos backfill) are presented in /Johannesson et al. 2010/.

The swelling pressure of the backfill is a function of all the variables included in the Table 4-7. Figure 4-6 shows example of results on different backfill materials /Johannesson and Nilsson 2006/.

Table 4-7. Direct dependencies between the process “Swelling/mass redistribution” and the defined tunnel backfill variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence? (How/Why not)	Influence present? (Yes/No) Description	Handling of influence? (How/Why not)
Temperature	Yes, affects thermal expansion and also indirectly via the hydro-variables	Excluded from the assessment, since the temperature increase is slow	(Insignificantly)	
Backfill geometry	Yes, 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 included in the modelling
Backfill pore geometry	Yes, through stress state and void ratio	Void ratio is included in the models	Yes, through stress state and void ratio	Void ratio is included in the models
Water content	Yes, decisive variable	Included in THM modelling of unsaturated backfill	Yes	Included in THM modelling of unsaturated backfill
Gas content	Yes, degree of saturation is a model variable	Included in THM modelling of unsaturated backfill	Yes, degree of saturation is a model variable	Included in THM modelling of unsaturated backfill
Hydro-variables (pressure and flows)	Yes, model variables	Included in THM modelling of unsaturated backfill	Yes, model variables	Included in THM modelling of unsaturated backfill
Stress state	Yes, model variable	Included in THM modelling of unsaturated backfills and included in calculation of the mechanical interaction with buffer	Yes, model variable	Included in THM modelling of unsaturated backfills and included in calculation of the mechanical interaction with buffer
Backfill materials – composition and content	Yes, influences the suction potential and the swelling pressure	The initial composition of the backfill is the starting point of the evaluation	No	
Backfill porewater composition	Yes, influences the suction potential and the swelling pressure	Included in the model via the suction potential and the swelling pressure etc	No	
Structural and stray materials	Yes	Not included in assessment	No	

Figure 4-7 shows the swelling pressure of IBECO-RWC-BF as a function of dry density at different conditions. Despite the scatter there is an obvious influence of porewater salinity and composition. The swelling pressure of MX-80 is shown in Section 3.4.1.

Influence of **degree of saturation and temperature** is the same as for the buffer; see Section 3.4.1.

The influence of the **stress state** expressed as compression properties is, together with the swelling pressure, important for the interaction with the buffer. Figure 4-8 shows, as an example, results from oedometer tests on different backfill candidates. The evolution of the dry density as a function of the applied stress is plotted /Johannesson and Nilsson 2006/.

The results in Figure 4-8 can be used for investigating the interaction between the backfill and the buffer and calculate the upwards displacement of the buffer/backfill interface.

The mechanical properties of the backfill blocks and the pellets filling before wetting are of special interest for modelling of the case with buffer swelling towards a dry tunnel backfill. Figure 4-9 shows examples of results from measurement of the strength of unwetted bentonite blocks at different dry densities.

Boundary conditions

The backfill has three main boundaries, namely the buffer, the rock and the plug at the end of the deposition tunnel.

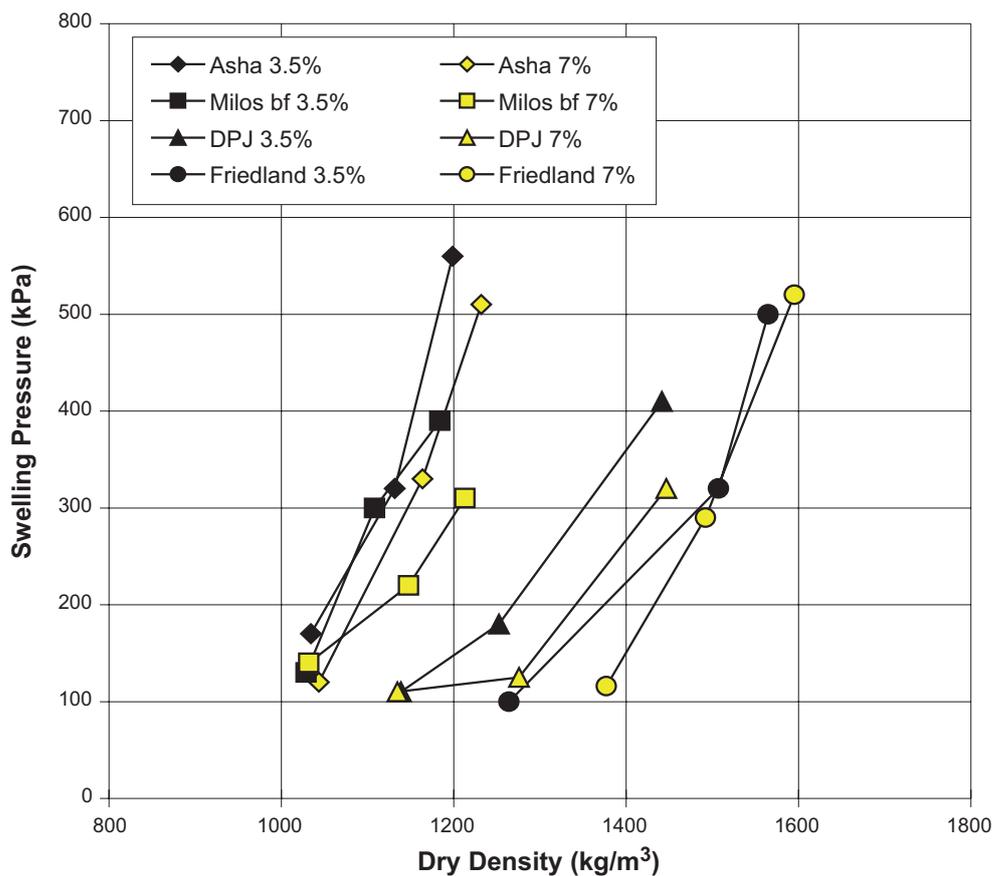


Figure 4-6. Swelling pressure of different backfill materials. The legend also shows the salinity of the water (50/50 CaCl/NaCl) /Johannesson and Nilsson 2006/.

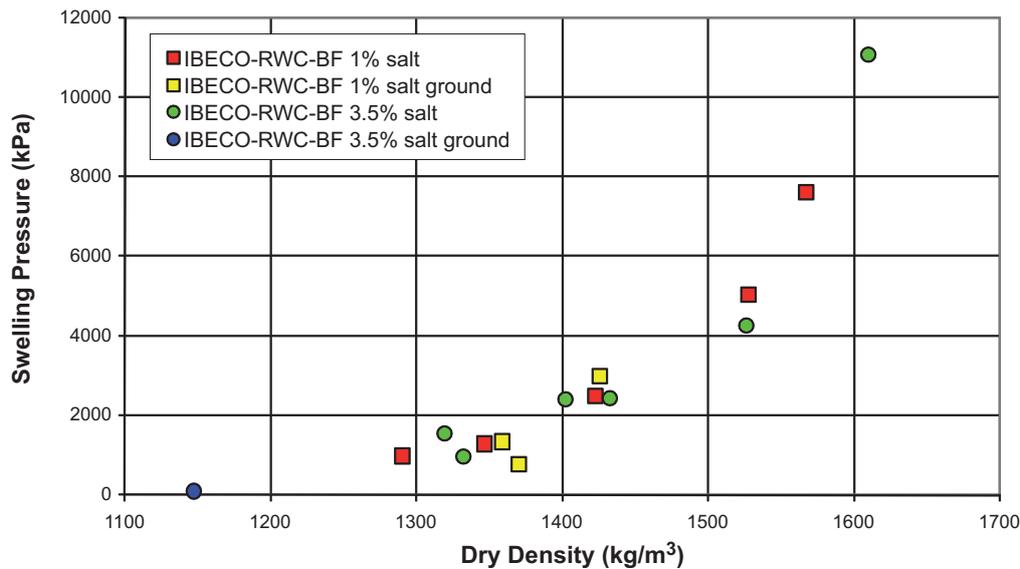


Figure 4-7. Swelling pressure of IBECO-RWC-BF as a function of dry density for the natural material and after grinding (legend: ground) at different porewater salinity /Johannesson et al. 2010/.

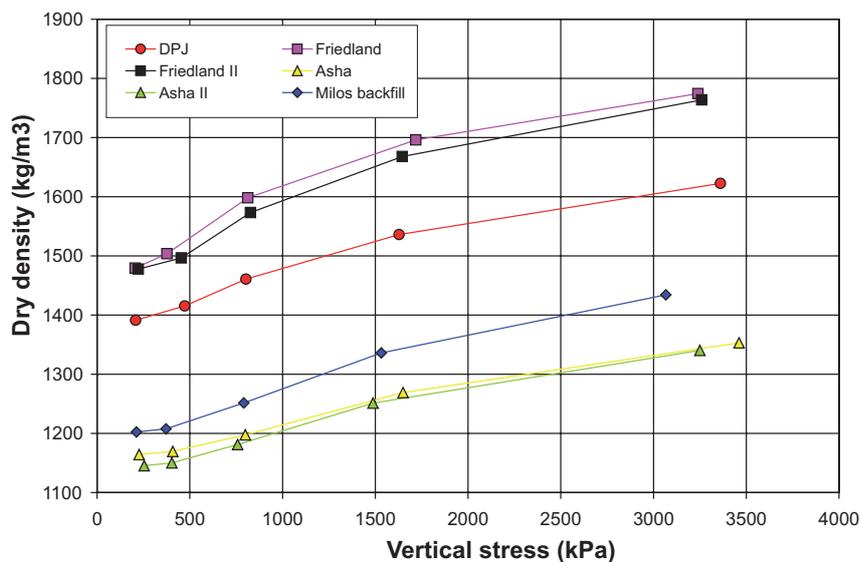


Figure 4-8. Evolution of the dry density as a function of the applied stress for different backfill candidates at different initial dry densities. Tests performed at full saturation /Johannesson and Nilsson 2006/.

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 swelling pressure is higher for the buffer than the backfill there is a positive net vertical pressure 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. An evaluation of the swelling of the buffer and corresponding compression of the backfill is provided in the buffer chapter (Section 3.4.1). The influence of the properties of the backfill has been investigated by /Johannesson 2008/ and by

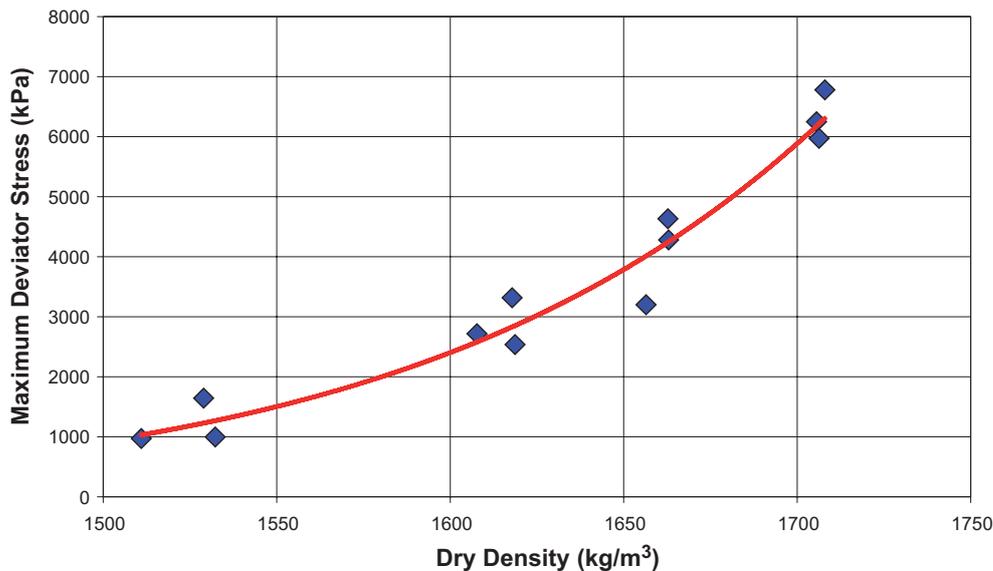


Figure 4-9. The deviator stress at failure as function of the dry density at unconfined compression tests made on IBECO-RWC-BF material. The water content is about 17% for all specimens /Johannesson et al. 2010/.

/Johannesson and Nilsson 2006/ with analytical calculations. In the former report also the effect of having a completely dry backfill when the buffer swells is analysed. Finite element calculations of these processes will be presented as a part of the SR-Site THM modelling /Börgesson and Hernelind 2009, Åkesson et al. 2010a/.

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 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 to support it in addition to the support according to item 1.
3. **Forces of friction** are developed between the backfill and the rock at the upper metre 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 means 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 buffer Section 3.4.1.

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 different backfill candidates have been investigated in the project “Backfilling and closure of the deep repository”. The results have yielded valuable information for estimating the required density of the backfill in the tunnels; see e.g. /Gunnarsson et al. 2006/ and /Keto et al. 2009/.

Laboratory tests on the mechanical properties of different backfill materials have been done (see e.g. /Sandén et al. 2008/ and /Johannesson et al. 2010/)

The only model studies done concerning mechanical processes in the backfill are the interaction buffer/backfill (see above and Section 3.4.1). Additional model studies will be done for SR-Site.

The mechanical properties of some of the backfill materials have been investigated /are not enough known today in order to make proper model calculations. Additional mechanical tests are planned.

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). However, these tests are of limited value since the backfill was composed of bentonite/sand mixtures and was in situ compacted. 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.

Self healing of backfill material lost by erosion needs to be confirmed. See also Sections 4.2.4 and 4.4.8.

Time perspective

Full saturation of the backfill and buffer is expected to be achieved within a couple of hundred years. This means that the stress equilibrium with full swelling pressure and fully developed swelling of the buffer against the backfill 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 been studied. Manmade bentonite seals are made in completely different ways (mixtures with low density) and natural bentonites have unknown histories. The existence of relevant natural analogues is probably very limited and difficult to evaluate.

Handling in the safety assessment SR-Site

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-Site is described in Section 3.4.1.

It is important to ensure that there is a tight connection between the backfill and the tunnel wall. This is achieved 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 4.4.6 and alterations of density, Sections 4.2.4, 4.4.8 and 4.4.7. The swelling pressure will be evaluated according to Section 3.4.1.

The initial swelling is modelled as part of the integrated initial THM evolution of the backfill /Åkesson et al. 2010a/. Also thermal expansion and interaction buffer/backfill is included in this modelling.

Homogenisation after loss of large masses of backfill after colloid erosion or plug disintegration is modelled for SR-Site /Åkesson et al. 2010a/.

The possible loss of backfill material expected during the installation and saturation phase is estimated as described in Sections 3.3.4 and 4.2.4. The channels and possible holes caused by the lost backfill are expected to be healed by swelling and homogenisation of the backfill (see e.g. /Johannesson et al. 2010/). Additional calculations in order to verify this will is done in the THM-modelling in SR-Site /Åkesson et al. 2010a/.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

The relation between swelling pressure and density for various bentonites and the influence of different factors as well as other mechanical properties are reported by e.g. /Karnland et al. 2006/, and /Johannesson et al. 2010/. These reports will undergo a documented factual- and quality review.

Modelling of backfill homogenisation (both the natural during the saturation phase and the sealing of erosion damages), buffer/backfill interaction and other mechanical effects on the backfill will be reported in a general THM modelling report that has been subjected to a documented factual- and quality review /Åkesson et al. 2010a/.

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 that are treated in Section 4.4.7.

Due to lack in good mechanical models of the lower range backfill material (as Friedland clay), the homogenisation and healing properties of these materials are uncertain.

Model simplification uncertainties in SR-Site

See corresponding process for the buffer (Section 3.4.1)

Input data and data uncertainties in SR-Site

See above. The relevant data uncertainties are discussed in the THM-data report /Åkesson et al. 2010b/.

4.3.2 Liquefaction

Overview/general description

Liquefaction is a process implying that a stiff material (soil) turns into liquid due to a disturbance of short duration.. 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. 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.

Handling in the safety assessment SR-Site

The process is neglected.

4.4 Chemical Processes

4.4.1 Advective transport of species

Overview/general description

In this context, advection refers to transport of any forms of additional matter, e.g. ions, molecules or colloids, with porewater flow. The transport direction is thereby principally from volumes of high water pressure to volumes of lower pressure. The process leads to redistribution of solutes in the porewater and thus affects the porewater composition. There are several possible causes of pressure

gradients in the tunnel backfill material, e.g. external water pressure, affinity for water in the bentonite and temperature induced volume change of the water. Advective transport is closely related to water flow in the tunnel backfill, which is described in Section 4.2.2. Advection may though be different from pure water flow due to ion equilibrium effects in the case of ions, and due to filtering by nano-sized pores in the case of colloids.

In principle, advective transport in the tunnel backfill material is governed by the same variables as in the buffer material (see Section 3.5.2). However, advective transport in the tunnel backfill material is expected to be higher than in the buffer since the backfill bentonite is of lower quality and that rock volumes with high water flow may be excluded for deposition holes. Still, the transport of solutes in the backfill is expected to be dominated by diffusion (see Section 4.4.2).

Dependencies between process and tunnel backfill variables

Table 4-8 summarises how the process influences and is influenced by all backfill variables and how these effects are treated in SR-Site.

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

See the description of the corresponding process in the buffer, Section 3.5.2 for general information. Specific tunnel material conditions may occur close to the roof and floor, mainly due to lower density at the roof interface and the interaction with the highly permeable disturbed zone in the floor caused by the rock excavation technique.

Natural analogues/observations in nature

See the description for the corresponding process in the buffer, Section 3.5.2.

Time perspective

Advective transport of solutes in the backfill may occur at all timescales.

Handling in the safety assessment SR-Site

Advective transport of species in the tunnel backfill is included in the integrated modelling of the chemical evolution of the near field (Section 3.5.6).

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 where the tunnel in question is situated 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 porewater is calculated.

Table 4-8. Direct dependencies between the process “Advective transport of species” and the defined tunnel backfill variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Backfill geometry	Yes, major importance	Included in transport modelling through hydraulic conductivity	Yes, minor effects possible through dissolution/precipitation	Neglected
Backfill pore geometry	Yes, major importance	Included in transport modelling through hydraulic conductivity	Yes, through dissolution/precipitation	Neglected
Temperature	Yes, through thermal expansion and viscosity	Effect is small and not considered in transport calculations	No, low flow rates	
Water content	Yes	Neglected since low water content will reduce the process	Yes, minor effects through dissolution/precipitation	Neglected
Gas content	Yes, reduced flow in unsaturated clay	Neglected since high gas content will reduce the process	Yes, through transport/precipitation of dissolved gas	Neglected
Hydro-variables (pressure and flows)	Yes, by definition	Included in transport modelling through hydraulic conductivity	Yes, minor osmotic and viscosity effects	Included in transport modelling
Stress state	Yes	Included in transport modelling through hydraulic conductivity	Yes, minor osmotic effects possible	Neglected
Backfill materials – composition and content	Yes, density through montmorillonite content.	Included in transport modelling through hydraulic conductivity	Yes, through dissolution/precipitation	Neglected
Backfill porewater composition	Yes, by definition	Included in transport modelling through hydraulic conductivity	Yes, by definition	Included in transport modelling
Structural and stray materials	Yes, as alternative transport paths	Neglected	Yes, through dissolution	Neglected

Uncertainties

Uncertainties in mechanistic understanding

The uncertainties in mechanistic understanding are the same as those for water transport under saturated condition for the buffer (Section 3.3.2). Model simplification uncertainties in SR-Site

Input data and data uncertainties in SR-Site

Input data for the study of hydraulic conductivity are primarily the empirical relationships between hydraulic conductivity and density, temperature and porewater composition. In SR-Site, this is handled by sensitivity studies with different hydraulic conductivities in the tunnels.

4.4.2 Diffusive transport of species

Overview/general description

An overview of diffusion processes and phenomena as relevant for the buffer is given in Section 3.5.3; these considerations also apply to a backfill consisting of low-grade bentonite (IBECO RWC-BF).

The importance of these processes for the backfill material considered here is difficult to quantify, because diffusion processes have not been studied in detail so far. 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 decreasing compaction/density (increasing pore size). In sand-bentonite mixtures EDL-effects are expected to be negligible (except at sufficiently high bentonite/sand ratios). In the proposed backfill of low-grade bentonite, the content of smectite is about 70%, (plus < 10% smectite/illite mixed layer) and a dry density of about 1,500 kg/m³ (clay fraction) is envisaged.

- Evidence from several different studies suggests that in case of material with a smectite content of about 95% to 45%, the overlap of EDL's leading to the so-called anion exclusion (see description of diffusion in the chapter on [processes in the buffer]) occurs at a dry density of about 1,200–1,500 kg/m³ /Kozaki et al. 1998/. At a dry density of 1,500 kg/m³, the porosity of Kunigel-V1 with a montmorillonite content < 50% is about 0.44; i.e. nearly identical to the foreseen porosity of the backfill. 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 will also be operative in IBECO RWC-BF clay under the foreseen conditions (porosity » 0.46).
- /Sato 1998/ gives a comparison of effective diffusivities for HTO and anions (Cl, I) for Kunigel-V1 Na-bentonite (dry density: 1,600 kg/m³) 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.
- /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/m³ for MX-80 as well as Kunigel-V1 bentonite, which has a smectite content of about 45%. Therefore, it can be assumed that this process may also play a role for the diffusive transport in the backfill. Note that enhanced cation diffusion is typically only relevant for Cs, because Cs is nearly always present in purely cationic form.
- 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.

Dependencies between process and tunnel backfill variables

Table 4-9 summarises how the process influences and is influenced by all backfill variables and how these effects are treated in SR-Site.

Influence of temperature, porewater composition and speciation, pore geometry, sorption:

Analogous to the relations discussed for the buffer in Section 3.5.3.

Influence 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 3.5.6, 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 4.4.4.

Boundary conditions

Limitation of the migration of major dissolved ions and radionuclide traces (remaining dissolved concentrations below the respective solubility limits) is analogous to the buffer. 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 into flowing water in the near-field fracture network (equivalent flow rate or Q_{eq}, see Section 3.6.2).

Table 4-9. Direct dependencies between the process “Diffusive transport of species” and the defined tunnel backfill variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Temperature	Yes	The temperature dependence of the diffusivity is not included in the transport calculations. The importance is regarded as small	No	
Water content	Yes.	Saturated conditions assumed.	No	
Gas content	Yes, by affecting pore space available for diffusion	Saturated conditions assumed.	No, but indirectly through porewater composition and dissolved gases such as CO ₂ or CH ₄ , which may come out of solution	
Hydro-variables (pressure and flows)	Yes.	Saturated conditions assumed	No	
Backfill geometry	Yes	Backfill dimensions are included in calculations	No	
Backfill pore geometry	Yes	Defines the magnitude of the diffusivities	No, but possibly indirectly through influence on porewater composition and swelling	
Stress state	No, but indirectly through pore geometry		No, but possibly indirectly through influence on porewater composition and swelling	
Backfill materials – composition and content	Through porewater composition	Defines the magnitude of the diffusivities	No, but indirectly through influence on porewater composition	
Backfill porewater composition	Extent of EDL depends on ionic strength	Defines the magnitude of the diffusivities	Through diffusive transport of main constituents	See 4.4.4
Structural and stray materials	Indirect on the geometry (through influence on physical pore width)		Possibly indirectly through influence on porewater composition	

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 specifically for IBECO RWC-BF.

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 (or transient) through-diffusion studies, which can directly yield D_e and porosity, are largely restricted to relatively mobile tracers (alkaline ions, HTO, anions) or low degrees of compaction. Few attempts have been made so far to derive diffusion coefficients through semi-mechanistic models. Some examples are discussed in Section 3.5.3 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-Site

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 4.4.4. 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 3.5.3. For the treatment of radionuclide diffusion, element-specific effective diffusivities are used together with corresponding porosities (see the SR-Site Data Report /SKB 2010I/).

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 4.4.4.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

Most general issues relevant for handling diffusion in the backfill are discussed in the sections 4.4.4 and 3.5.3. All radionuclide-specific data (effective diffusivities and porosities) are taken from SKB reports /Ochs and Talerico 2004/ and SR-Site Data Report /SKB 2010I/ dedicated to the derivation of system-specific data that are consistent with the specified properties of IBECO RWC-BF Sets of diffusion-available porosities and effective diffusion coefficients are selected / for anions, cations (essentially Cs) and elements existing largely as neutral species (on average) under the relevant pore-water conditions. To define selected parameter sets, a large amount of original experimental data, published in peer-reviewed journal articles and proceedings and in reviewed reports, was evaluated.

Uncertainties

Uncertainties in mechanistic understanding

Uncertainties in mechanistic understanding of diffusion in compacted, expandable clay materials are discussed in Section 3.5.3 this discussion applies also to the case of backfill.

Model simplification uncertainties for the above handling in SR-Site

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 4.4.4 and 3.6.2). In that sense, the diffusion input parameters have to be viewed as conditional; i.e. their application will only be valid under the conditions (in particular backfill density) 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-Site

Input data to SR-Site are effective diffusivities and diffusion-available porosities to be directly used in consequence calculations. Data and uncertainties for IBECO RWC-BF are accepted from /Ochs and Talerico 2004/; after scaling to the specified reference density.

4.4.3 Sorption (including exchange of major ions)

Overview/general description

An overview of sorption and ion exchange processes relevant for the buffer is given in Section 3.5.5. Since the current backfill material is similar to the buffer in most respects, the process can be treated in the same fashion.

Dependencies between process and tunnel backfill variables

Table 4-10 summarises how the process influences and is influenced by all buffer variables and how these effects are treated in SR-Site.

Influence of backfill and porewater composition, and of temperature: Analogous to the situation of the buffer (see Section 3.5.5).

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.

Table 4-10. Direct dependencies between the process “Sorption (including exchange of major ions) and the defined tunnel backfill variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Backfill geometry	No	(Total backfill mass considered)	No	
Backfill pore geometry	No, but possibly indirectly through influence on EDL properties		No, but possibly indirectly through influence on EDL properties/swelling	See 3.5.5
Temperature	Yes	Influence of temperature on sorption must be acknowledged, but effect is not clear	No	
Water content	No, but indirectly through porewater composition		No	
Gas content	No, but indirectly through porewater composition (CO ₂)		No, but possibly indirectly through influence of Ca-exchange on carbonate equilibria	See 3.5.5
Hydro-variables (pressure and flows)	No, but indirectly through porewater composition		No, but possibly indirectly, through porewater composition/swelling	See 3.5.5
Stress state	No, but indirectly through influence on porewater composition and EDL properties		Indirectly through influence on porewater composition and EDL properties	See 3.5.5
Backfill materials – composition and content	Yes	Chemical data used for sorption coefficient estimates	(Surface composition)	See 4.4.4
Backfill porewater composition	Yes	Chemical data used for sorption coefficient estimates	Yes	See 4.4.4
Structural and stray materials	Yes	Sorption on stray materials is conservatively excluded in SR-Site	Indirectly through influence on porewater composition and related mineral equilibria	

Boundary conditions

Analogous to the situation of the buffer (see Section 3.5.5).

Model studies/experimental studies

Analogous to the situation of the buffer (see Section 3.5.5).

Time perspective

Analogous to the situation of the buffer (see Section 3.5.5).

Natural analogues/observations in nature

Analogous to the situation of the buffer (see Section 3.5.5).

Handling in the safety assessment SR-Site

Before saturation: Sorption of radionuclides is neglected before saturation since there is no continuous water path available. The geochemical evolution of the backfill during saturation is not considered in SR-Site.

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” in the description of process Alterations of backfill impurities, Section 4.4.4.

Failed canister: Sorption is included in the modelling of radionuclide transport for the long-term phase, see heading “Handling” for process 3.6.1 As for the buffer, sorption is treated through element-specific K_d values derived for specific conditions (see /Ochs and Talerico 2004/ and the SR-Site Data Report /SKB 2010/ 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 calculations. Because of the conditional nature of K_d , the data selected are derived for conditions expected to be relevant for safety assessment 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 4.4.4; these processes are also taken into account in the derivation of radionuclide K_d values.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

Most general issues relevant for handling ion exchange of major ions and radionuclide sorption are discussed in Sections 4.4.4 and 3.6.2. As in the case of radionuclide sorption in the buffer, all radionuclide-specific data are taken from a SKB report /Ochs and Talerico 2004/ specifically dedicated to the derivation of diffusion and sorption coefficients. That report was subjected to a factual review according to the standard for the SR-Can project. Distribution coefficients were calculated by /Ochs and Talerico 2004/ on the basis of a porewater composition calculated for a specified clay-groundwater interaction scenario. As source data for the derivation of scenario-specific distribution coefficients, a large amount of original experimental data, published in peer-reviewed journal articles, proceedings and reports, was evaluated. In a few cases, calculations with thermodynamic sorption models were carried out for comparison. The sorption data to be used in the radionuclide transport calculations are qualified in the SR-Site Data report /SKB 2010/.

Uncertainties

Uncertainties in mechanistic understanding

The discussion given for the corresponding process in the buffer (Section 3.5.5) is also applicable to the backfill.

Model simplification uncertainties in SR-Site

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. 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 in SR-Site

Input data to SR-Site 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. The sorption data to be used in the radionuclide transport calculations are qualified in the SR-Site Data report /SKB 2010/.

4.4.4 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 3.5.6).

The main differences are:

1. The temperature in the backfill is 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. However, the IBECO-RWC-BF is geochemically rather similar to the Deponit CA-N (IBECO-RWC) buffer material, since they originate from the same deposit.
3. Both advective and diffusive transport of species may be active in the backfill.

Dependencies between process and tunnel backfill variables

Table 4-11 summarises how the process influences and is influenced by all backfill variables and how these effects are treated in SR-Site.

Temperature: Thermodynamic constants of chemical reactions are highly dependent of the temperature. However, the maximum expected temperatures in the backfill are around 40°C during the first 100 to 200 years (see Section 4.1.1). Although even at these temperatures some changes can occur, the overall effect is likely to be less critical here than in the buffer.

Table 4-11. Direct dependences between the process “Alterations of backfill impurities” and the defined tunnel backfill variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Backfill geometry	Yes, the total amount of minerals in the backfill and the bentonite/porewater ratio affects the process	The geometry and the bentonite mass, as well as the bentonite/porewater ratio is considered in the model	No	
Backfill pore geometry	No, but indirectly through porewater composition	Determines the diffusivity see 4.4.2, which is considered in the model.	Precipitation-dissolution of minerals	Included in model but of minor concern in backfill
Temperature	Yes. 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	No, but indirectly through effects on solute transport and porewater composition.	However, the chemical model assumes saturated conditions	No	
Gas content	No, but indirectly through dissolution of gas and porewater composition.		Yes	Dissolved gases are included in the model
Hydro-variables (pressure and flows)	No, but indirectly through porewater composition	Darcy flow is included in the model, see 4.4.1	No	
Stress state	Yes	Partial pressures of gases are included in model	Yes	The results from the model is evaluated to consider effects on swelling pressure
Backfill materials – composition and content	Yes	Composition data is considered in model	Yes	The evolution of the composition is calculated with the model
Backfill porewater composition	Yes	Composition data is considered in model	Yes	The evolution of the composition is calculated with the model
Structural and stray materials	No, but indirectly by affecting porewater composition.	See 4.4.7	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-Site

Water content: The effect of water content on the alteration of accessory minerals is indirect. As the saturation process affects the transport of solutes, this in turn affects the chemical reactions. Therefore the water saturation process can result in significant changes in the redistribution of accessory minerals and on the chemical composition of porewater. Precipitation-dissolution of accessory minerals can result in minor changes of porosity, and therefore to the water-solid ratio or available porosity for water uptake. However, this change in porosity is expected to be very small.

Gas content: The formation of a gas phase can modify the concentration of solutes in the porewater, and therefore to the stability of accessory minerals. However, this process is expected to be very limited in the backfill.

Hydrovariables (pressure and flows): Transport of dissolved chemical species in the system can modify the dissolution-precipitation rates of accessory minerals by maintaining the saturation state of these phases far from equilibrium.

Backfill geometry: The geometry of the backfill can affect indirectly the alteration of accessory minerals through the transport processes associated to the solutes in the groundwater and bentonite porewater, thus affecting the behaviour of geochemical reactions during its interaction. Moreover, the backfill geometry determines the total pool of accessory minerals able to react in the system due to the interaction of groundwater and bentonite.

Backfill pore geometry: The pore geometry of the backfill affects the transport of solutes modifying the chemical composition of porewater within the backfill and hence, affecting the geochemical reactions taking place in the backfill. In addition, precipitation-dissolution of accessory minerals can modify the porosity distribution in the backfill as well as the pore geometry.

Stress state: The increase in the partial pressure of gases can affect the stress in the system. The build up of such partial pressures could be a direct consequence of the alteration of impurities. However, as gas phases are not expected to form in the backfill, the influence of this variable is expected to be negligible.

Backfill composition: This is one of the most relevant variables influencing the alteration of impurities. The type and amount of accessory minerals and montmorillonite is essential to determine how their dissolution-precipitation behaviour will affect the chemical evolution of the system. Moreover, the dissolution-precipitation of these mineral phases will modify the bentonite composition during the interaction with porewater. The composition of montmorillonite, especially the cation exchanger (type of cations and occupancy) is very relevant, as the interaction with backfill porewater will modify the chemical composition of this porewater and, hence, the dissolution-precipitation of accessory minerals in the bentonite. In addition, the alteration of bentonite impurities will modify the chemical composition of bentonite porewater and hence the montmorillonite composition.

Backfill porewater composition: The porewater composition will determine which of the accessory minerals in the bentonite will dissolve or precipitate, and thus the dissolution-precipitation of these minerals will modify the chemical composition of porewater.

Structural and stray materials: The interaction of bentonite porewater with structural and stray materials can result in the modification of the chemical composition of porewater and, therefore, in the behaviour of accessory minerals and vice versa.

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-Site. Some of the work done with buffer materials is of relevance for the backfill as well (Section 3.5.6).

Natural analogues/observations in nature

Some of the work done for buffer materials may be of relevance for the backfill as well (Section 3.5.6).

Time perspective

The process is relevant for the whole assessment period.

Handling in the safety assessment SR-Site

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. No specific modelling of the geochemical evolution in the backfill for the saturation phase will be done.

Thermal period: The thermal effects on the chemical evolution of the backfill are not included in SR-Site, since the temperature elevation and the thermal gradients are small.

After saturation: The process is included in the scenario-specific modelling of the backfill chemical evolution for the post-thermal long-term phase. The model considers advection, diffusion, ion-exchange and mineral dissolution/precipitation in the backfill compartment. Figure 4-10 shows an example from the modelling of the pH evolution in the backfill together with calcite and gypsum content and calcium occupancy in the exchanger of the backfill. pH in the backfill is buffered by calcite precipitation-dissolution, which in turn is affected by calcium availability due to cation exchange processes. As exchange reactions reach 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 is obtained, decreasing the pH of porewater 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 was not included in the model mentioned above, although it is envisaged to be included in future modelling exercises.

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 Q_{eq} 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 (porewater 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 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 3.5.9.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

No separate references are used for the backfill. However, the geochemical processes are the same as for the corresponding process in the buffer. Therefore, the same references apply (see Section 3.5.6).

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.

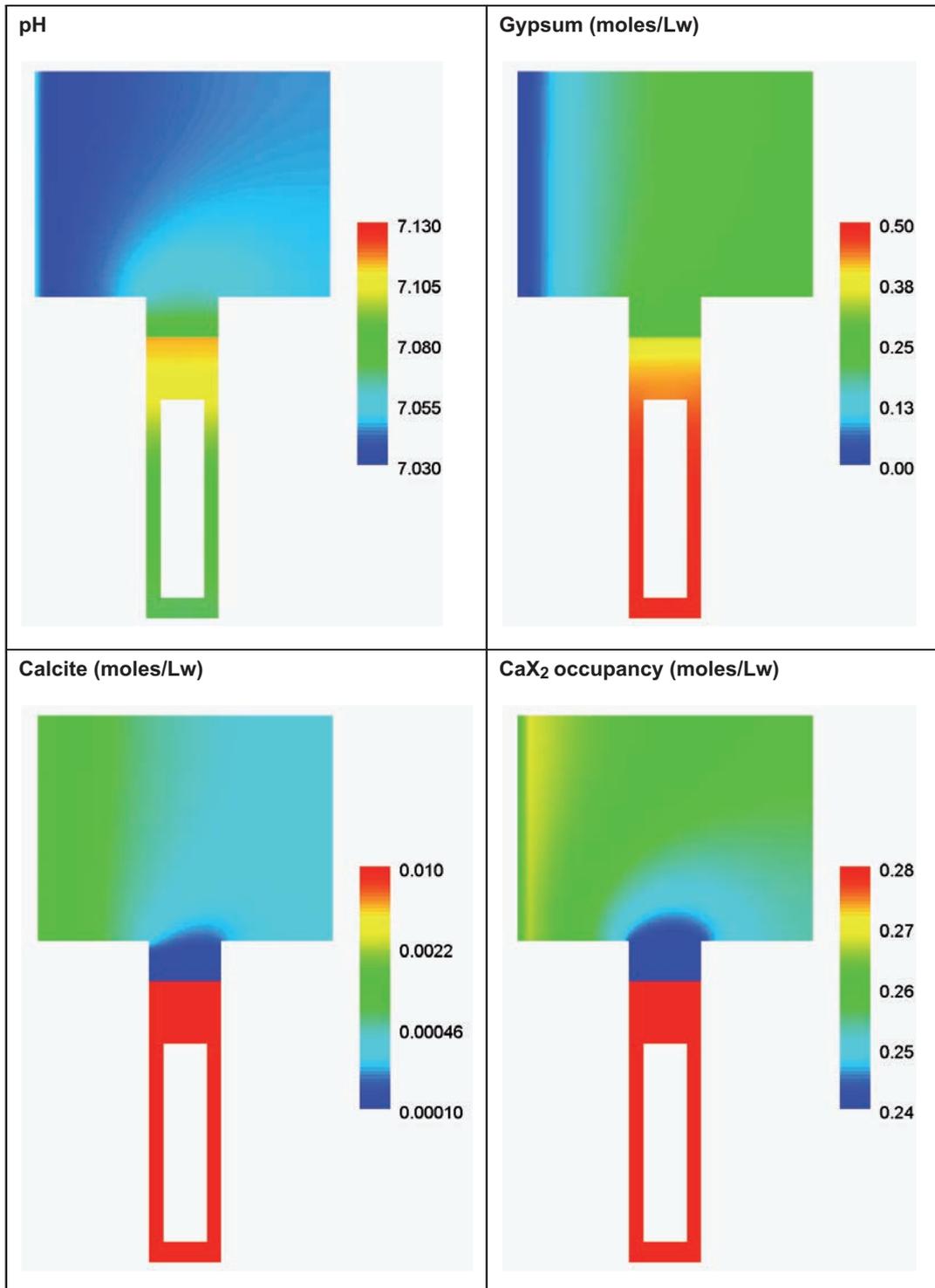


Figure 4-10. Graphics showing the predicted evolution in the simulated domain (Deponit CA-N bentonite buffer and Friedland backfill) for pH, calcite and gypsum content and calcium occupancy in the cation exchanger of montmorillonite after 60,000 years of simulation. Groundwater is simulated to enter the system through a conductive fracture perpendicular to the deposition gallery at the left boundary of the domain (units in moles per litre of porewater). Note that as gypsum dissolves both calcium occupancy in the exchanger and calcite content increase and pH slightly decreases in the backfill /Arcos et al. 2006/.

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 in SR-Site

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 porewater, thus affecting the chemical long-term evolution of the bentonite. See also Section 3.5.9.

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 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 these 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 initial accessory mineral pool. Thus the effect of dissolution/precipitation of these minerals on the master variables will be assessed.

Input data and data uncertainties in SR-Site

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-Site data report.

4.4.5 Aqueous speciation and reactions

Overview/general description

This process is in general identical with the corresponding process in the buffer (Section 3.5.7)

Handling in the safety assessment SR-Site

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 backfill chemical evolution for the thermal phase and the post-thermal long-term phase. This is described in Section 4.4.4.

Failed canister: The backfill is assumed to be unaffected geochemically from the canister insert. However, the properties of the backfill are considered in the radionuclide transport calculations.

4.4.6 Osmosis

Overview/general description

The general principle for this process is the same as for the corresponding buffer process (Section 3.5.8). 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 has to balance the swelling pressure from the buffer.

Dependencies between process and tunnel backfill variables

Table 4-12 summarises how the process influences and is influenced by all backfill variables and how these effects are treated in SR-Site.

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 3.5.8).

Natural analogues/observations in nature

The study reported in the buffer section is relevant also for the tunnel backfill (Section 3.5.8).

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-Site

The effects of the ionic strength of the groundwater on the hydraulic properties of the backfill are handled by direct application of empirical data mainly given in /Karlund et al. 2006/.

Table 4-12. Direct dependencies between the process “Osmosis” and the defined tunnel backfill variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence? (How/Why not)	Influence present? (Yes/No) Description	Handling of influence? (How/Why not)
Backfill geometry	No		Yes, possible at low backfill density	Empirical assessment
Backfill pore geometry	Yes, interlayer distance is a decisive parameter	The density is given as initial condition	Yes, rearrangement of pore sizes at extreme conditions	Empirical assessment
Temperature	Yes, linear dependence	Neglected due to small differences in temperature	No	
Water content	Yes, equivalent to pore geometry in saturated backfill	Saturated conditions assumed	Yes, possible at low backfill density	Neglected
Gas content	No, the process is not well defined in unsaturated backfill		No	
Hydrovariables (pressure and flows)	No, only indirectly since flow may modify ion equilibrium		Yes, hydraulic conductivity effects	Empirical assessment
Stress state	No, only indirectly through charge compensating cation concentration		Yes, by definition	Empirical assessment
Backfill materials – composition and content	Yes, through montmorillonite content. Number and type of charge compensating cations are of decisive importance	Empirical assessment	No	
Backfill porewater composition	Yes, by definition	Empirical assessment	Yes, by definition. Governs the interlayer ion concentration	Of no concern
Structural and stray materials	No		No	

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.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

The principles for osmosis, ion equilibrium (Donnan equilibrium) and the resulting pressure effects are basic knowledge in physical chemistry, and are consequently supported by numerous peer reviewed articles available in the open literature. The coupling to bentonite buffer systems is shown in /Karlund et al. 1997/ and /Karlund et al. 2006/. Both are SKB reports and the latter undergo documented factual- and quality review at present. /Karlund et al. 2005/ is not an SKB report, but is developed within the framework of a quality assurance system that requires a documented factual- and quality review before approval and printing and is available in the open literature. The natural analogue support for osmosis /Neuzil 2000/ is a peer reviewed article (Nature) that is available in the open literature.

Uncertainties

The uncertainties are the same as those for the buffer (see Section 3.5.8) except for a larger uncertainty in the theoretical calculations of pressure effects due to the larger amount of accessory minerals in the low grade bentonite.

4.4.7 Montmorillonite transformation

Overview/general description

The general principle for this process is the same as for the corresponding buffer process (Section 3.5.9). 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 than 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.

Dependencies between process and tunnel backfill variables

Table 4-13 summarises how the process influences and is influenced by all backfill variables and how these effects are treated in SR-Site.

Boundary conditions

See the corresponding buffer process; Section 3.5.9).

Model studies/experimental studies

The studies reported in the buffer section are relevant also for the tunnel backfill (see Section 3.5.9).

Natural analogues/observations in nature

The studies reported in the buffer section are relevant also for the tunnel backfill (see Section 3.5.9).

Time perspective

Significant transformation is not expected during the lifetime of the repository according to the kinetic model for illitisation.

Handling in the safety assessment SR-Site

The alteration of the swelling component in the backfill could be treated in the same way as for the buffer (Section 3.5.9). The only difference is the maximum temperature and the amount of material. Since the temperature is low under all conditions, montmorillonite alteration, in the form of illitization, can be neglected in the backfill. It is also assumed that the cement in the repository will be of the “low-pH” type and will have insignificant impact on the properties of the backfill.

Table 4-13 . Direct dependencies between the process “Montmorillonite transformation” and the defined tunnel backfill variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Backfill geometry	Yes, determines total mass available, indirectly through transport of dissolved species	Included in evaluation	Yes at extreme transformation	–
Backfill pore geometry	No, indirectly through transport of dissolved species and ion equilibrium		Yes, direct consequence	Included in transformation evaluation
Temperature	Yes, major impact	Included in transformation expression	No	
Water content	No, indirectly through transport of dissolved species and ion equilibrium	No credit taken	Yes, possible but not necessary	
Gas content	No, indirectly through water content		No	
Hydrovariables (pressure and flows)	Yes, controls supply of dissolved species (mass balance)	Included in transformation evaluation	Yes, change in hydraulic conductivity	Effect on hydraulic conductivity can be evaluated
Stress state	No, pressures are to small		Yes, direct consequence	Loss of swelling is evaluated as a case with a high conductivity backfill
Backfill materials – composition and content	Yes, through available species in accessory minerals	Included in transformation expression	Yes, by definition	Included in transformation expression
Backfill porewater composition	Yes, major impact	Included in transformation expression	Yes, major impact	Only effects on the backfill itself are considered
Structural and stray materials	No, but indirectly through porewater and dissolved species. Especially pH effects from cement	Discussed in the buffer alteration scenario.	No	

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

Montmorillonite alteration is one of the most studied processes in clay mineralogy and the above argumentation is supported by numerous peer reviewed articles and conference papers that are available in the open literature. The above cited ones represent only a minor fraction of what is available and the key issues are rather the relevance and relative quality of the peer reviewed material. A literature study with special respect to KBS-3 conditions including a validation of alteration models, especially quantitative, was made by SKB /Karland and Birgersson 2006/ in order to address these issues. This report may be seen as a comprehensive exposition of the adequacy of references.

Uncertainties

The uncertainties are the same as for the corresponding buffer process (Section 3.5.9).

4.4.8 Backfill 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). The same principles are valid for the backfill system as for the buffer (see section 3.5.11) with the following exceptions.

Deposition holes will not be placed in rock volumes with larger fractures or severe groundwater flow. The option to fully avoid such zones may not be present in the placement of deposition tunnels. The tunnel backfill material may thereby be exposed to more adverse conditions than the buffer material both with respect to fracture apertures and flow rates.

The tunnel backfill material will have lower content of montmorillonite or other swelling minerals compared to the buffer material. Colloid release leads to replacement of lost montmorillonite by swelling of the remaining montmorillonite, which leads to a successive deterioration of the sealing properties. In principle, high quality bentonite materials will thereby stay relatively homogeneous and the sealing properties will decrease generally but slowly. In contrast, accessory minerals in low quality bentonite materials may serve as a filter and prevent replacement of lost material. This potential filter effect may reduce the loss of montmorillonite, but it may also lead to high local hydraulic conductivity in the depleted part of the backfill. The content and the grain size distribution of the accessory material will determine the extent of such a filter function.

Dependencies between process and tunnel backfill variables

Table 4-14 summarises how the process influences and is influenced by all backfill variables and how these effects are treated in SR-Site.

Table 4-14. Direct dependencies between the process “Colloid release” and the defined tunnel backfill variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence? (How/Why not)	Influence present? (Yes/No) Description	Handling of influence? (How/Why not)
Backfill geometry	Amount of backfill present	Included in modelling	Yes, at extreme colloid release	Included in modelling
Backfill pore geometry	Yes, governs the dispersing forces	Included in modelling	Yes, by definition	Included in modelling
Temperature	No, negligible		No	
Water content	Yes, by definition	Included in modelling	Yes, by definition	Included in modelling
Gas content	Yes, no dispersion possible from unsaturated clay	Boundary condition	No	
Hydrovariables (pressure and flows)	Yes, groundwater flow may determines the mass loss	Included in modelling	Yes, indirect through pore geometry, central impact	Evaluated from modelling results
Stress state	Yes, by definition	Included in modelling	Yes, major impact	Included in modelling
Backfill materials – composition and content	Yes, impurities may govern the ion type and concentrations	Included in modelling	Yes, selective loss of the montmorillonite content	Included in modelling
Backfill porewater composition	Yes, major importance both with respect to cation type and concentration	Included in modelling	No, but indirectly through pore geometry which affects the counterion concentration	Included in modelling
Structural and stray materials	No, but indirectly through porewater composition. Especially concrete may support with calcium ions		Indirectly, a minor effect of calcium uptake from cement structures could be imagined	

Boundary conditions

The boundary conditions are the same as for the corresponding buffer process; see Section 3.5.11

Model studies/experimental studies

All studies reported in the buffer section on colloid release are relevant also for the tunnel backfill (Section 3.5.11).

Natural analogues/observations in nature

All studies reported in the buffer section are relevant also for the tunnel backfill (Section 3.5.11).

Time perspective

Colloid release is only possible at low ion concentrations and likely only relevant in conjunction with glaciations. The effects will be significant only in the long-term perspective.

Handling in the safety assessment SR-Site

The handling of the process is the same as for the corresponding process in the buffer (Section 3.5.11). The main difference is that the total mass of backfill is much larger than of the buffer.

Uncertainties

The uncertainties are the same as for the corresponding buffer process (Section 3.5.11).

4.4.9 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 (see Section 3.5.12).

Handling in the safety assessment SR-Site

The process is neglected since the dose rate in the tunnel backfill is too low to have any effects (see Section 3.5.12).

4.4.10 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 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 are thoroughly discussed in the Geosphere process report /SKB 2010i/. 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 been discussed elsewhere in this report (Section 3.5.14). Those processes are expected to be limited to an initial phase, after which temperature, radiation, desiccation and the swelling pressure are assumed to sterilise the buffer /Pedersen 2002/. The radiation, desiccation and the swelling pressure limiting effects on microbial processes in the backfill will be less

pronounced or as good as absent with respect to radiation, and continued microbial activity will be possible. On the other hand, the consequences of microbial activity is rather positive than negative in this part of the repository because of the oxygen reducing and redox-lowering effects caused by most active microorganisms.

Dependencies between process and tunnel backfill variables

Table 4-15 summarises how the process influences and is influenced by all backfill variables and how these effects are treated in SR-Site.

Table 4-15 . Direct dependencies between the process “Microbial processes” and the defined tunnel backfill variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Backfill geometry	No		No	
Backfill pore geometry	No		Growth of microbes generate biomass that may clog pores	Neglected due to limited amounts of organic carbon
Temperature	Yes Most microbes have an ideal temperature range in which they thrive. Maximum temperature for life is 113°C.	The microbial effects are treated with a mass-balance.	No	
Water content	Yes Water is needed for active life.	Full saturation is assumed	No	
Gas content	Yes Hydrogen and methane can be consumed by microbes that will grow and produce biomass; largest effect is obtained if oxygen is present. Some microbes produce acetate with hydrogen and carbon dioxide	The microbial effects are treated with a mass-balance.	Microbes both produce and consume gases	Neglected, since gas in the backfill is of limited concern
Hydro-variables (pressure and flows)	No		Yes Gas pressure may lead to advective flow	Neglected, since extent is limited
Stress state	No		No	
Backfill materials – composition and content	Organic impurities will have an effect	The microbial effects are treated with a mass-balance.	No	
Backfill porewater composition	Microbes are sensitive to the geochemical situation, and may utilise porewater components for growth	The microbial effects are treated with a mass-balance.	Microbial activity may change the composition, e.g. by consumption of methane, sulphate and organic carbon and production of acetate, sulphide and carbon dioxide	The possibility of microbial reactions will be considered. See 3.5.14
Structural and stray materials	Organic parts of this material and hydrogen from corroding metal will be a source of carbon and energy for microbes with growth as the result.	The microbial effects are treated with a mass-balance.	Microbes may oxidise organic components in this material and hydrogen from anaerobic corrosion.	The microbial effects are treated with a mass-balance. However, these materials serve no long term function

Boundary conditions

The access to metals and organic material, e.g. stray materials, including hydrogen from anaerobic corrosion of iron, e.g. rock bolts and armouring and methane and electron acceptors /SKB 2010i/ will set the limits for microbial process rates in the backfill.

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 of the Backfill & Plug Test, the survival and activity of added as well as naturally occurring microbes in the backfill will be analysed. However, this material is no longer considered as tunnel backfill. The studies on pure bentonite discussed for the buffer processes will represent the backfill quite well, as it will consist of bentonite only.

In addition, analyses 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. The results showed presence of micro-organisms in the porewater and demonstrated that porewater gases such as methane and hydrogen have increased significantly in concentration in the gas phase since closure /Eriksson 2007/.

Natural analogues/observations in nature

There is a natural analogue in Dunaorobba, 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 backfill have been summarised in a conceptual model as follows /confer Figure 3-5 in Pedersen 2000/. 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. There will also be spores and microorganisms in the backfill that can grow when water becomes available. 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-Site

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.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

All the references in this section are from peer reviewed scientific journals.

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 in buffer material.

Model simplification uncertainties in SR-Site

The effects of microbial reactions are maximised since a mass-balance expression is used.

Input data and data uncertainties in SR-Site

The amount and availability of organic materials and metals in the backfill and its vicinity will determine the extent of microbial reactions. The range of data can be found in /the Backfill Production Report /SKB 2010e/.

4.5 Radionuclide transport processes

4.5.1 Speciation of radionuclides

Overview/general description

See the corresponding buffer process; Section 3.6.1.

Handling in the safety assessment SR-Site

The handling of the process is the same as for the corresponding process in the buffer (see Section 3.6.1.). Data and boundary conditions for the backfill will be used.

4.5.2 Transport of radionuclides in the water phase

Overview/general description

See the corresponding buffer process; (Section 3.6.2).

Handling in the safety assessment SR-Site

The handling of the process is the same as for the corresponding process in the buffer (see Section 3.6.2). Data and boundary conditions for the backfill will be used.

5 Processes in the tunnel plugs

5.1 Thermal processes

5.1.1 Heat transport

Overview/general description

Tunnel plugs are typically located some 6 m from the outermost canister in each tunnel /SKB 2009b/. The plug volumes are sufficiently small that the temperatures are controlled by the temperature of the surrounding rock, meaning that the plug temperatures can be calculated without account of the heat transporting properties of the plug material. Therefore, the process is without significance to the thermal evolution in the plug region. Figure 5-1 shows the temperature at four points in the tunnel plug region as function of time, calculated using the analytical method described in /Hökmark et al. 2009/. Temperatures are at most about 28°C above the initial conditions. The peak occurs some 300 years after deposition. The temperature gradients are small vertically as well as horizontally. The maximum, at early times, is about 0.7°C/m.

Dependencies between process and tunnel plug variables

Table 5-1 summarises how the process influences and is influenced by all tunnel plug variables and how these effects are treated in SR-Site.

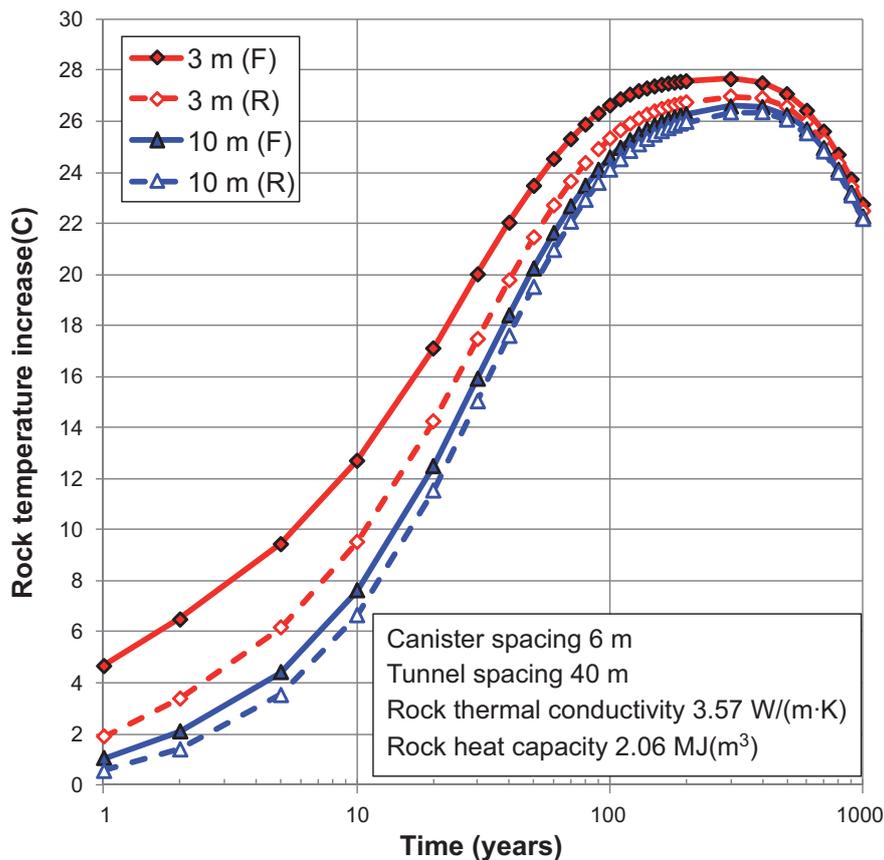


Figure 5-1. Temperature increase at 3 and 10 m distances from the outermost canister in a tunnel. Results shown are for two elevations: Tunnel floor (solid lines) and tunnel roof (dashed lines). Results obtained using calculation scheme described in /Hökmark et al. 2009/.

Table 5-1. Direct dependencies between the process “Heat transport” and the defined tunnel plug variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Plug geometry	No		No	
Pore geometry	Yes	Process neglected. Of no significans for the thermal evolution compared to other processes.	Indirectly via tempearture	Process neglected. Of no significans for the thermal evolution compared to other processes.
Temperature	Yes Heat transport is slightly temperature dependent.	Process neglected	Yes. But insignificant . (Controlled by rock temperature).	Process neglected
Water content	Yes. Thermal conductivity of the plug	Process neglected	No	
Gas content	No, but indirectly via water content		No	
Hydrovariables (pressure and flows)	No		No, but indirectly via temperature	Process neglected
Stress state	No		No, but indirectly via temperature	Process neglected
Plug materials – composition and content	Yes Composition affects thermal conductivity	Process neglected	No	
Porewater composition	No		No	

Plug geometry: The plug geometry is not important to the heat transport within the plug or to the plug temperature. The plug temperature is controlled by the slowly varying boundary conditions, i.e. the temperature of the rock surrounding the plug. Heat transport does not influence the geometry.

Plug pore geometry: The pore geometry may influence the transport properties but since plug heat transport does not control the plug temperatures, this is of no importance. The temperature may influence the pore geometry, but this is not controlled by the plug heat transport.

Temperature: Heat transport influences the temperature by definition. For the plug, however, it is the heat transport in the surrounding rock that controls the temperature. Any temperature dependences of the plug heat transport properties are unimportant.

Water content: The heat transport will not affect the water content, other than indirectly via the temperature. However, the temperature is determined by heat transport in the rock, not by the plug heat transport. Similar to the backfill, the plug thermal conductivity depends on the water content, but since plug heat transport does not impact on anything related to the safety assessment, there is no reason to quantify the content-conductivity relation.

Gas content: Same as above for the water content.

Hydro variables: None of the hydrovariables depend on the heat transport.

Stress state: The temperature increase will reduce or decrease the stresses in the plug, depending on whether the volume expansion of the plug material is smaller or larger than that of the rock. The temperature is controlled by the rock temperature, not by the heat transport within the plug.

Plug composition: The composition of the plug will influence the thermal conductivity. Some minerals have higher conductivities than others.

Plug porewater composition: The composition cannot influence the heat transport. The temperature, but not the heat transport within the plug, may promote chemical reactions.

Boundary conditions

The rock walls and the tunnel backfill are boundaries with slowly varying temperatures which are completely determined by the overall thermal evolution of the rock mass.

Model studies/experimental studies

There are no model studies that explicitly address the thermal conditions in tunnel plugs.

Natural analogues/observations in nature

Not applicable.

Time perspective

The duration of the thermal pulse generated by the decaying fuel is a few thousand years.

Handling in the safety assessment SR-Site

There is no specific handling of heat transport in the tunnel plugs.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

Because of the small thermal gradients and the relatively low temperatures in the tunnel plugs there is no specific handling of the heat transport process. The gradient and temperature statements are supported by results obtained using calculation schemes described in /Claesson and Probert 1996/. While this particular report is not peer or factual reviewed, the calculation scheme has been repeatedly applied in peer reviewed papers /Hökmark and Claesson 2005/ and in reports that have undergone (/Hökmark and Fälth 2003/) or will undergo (/Hökmark et al. 2009/) a documented factual and quality review.

Uncertainties

Uncertainties in mechanistic understanding

There are no major uncertainties in the mechanistic understanding of the heat transport in tunnel plugs.

Model simplification uncertainties in SR-Site

Not relevant since the process is not modelled.

Input data and data uncertainties in SR-Site

Not relevant since the process is not modelled.

5.1.2 Freezing

Overview/general description

Freezing of the tunnel plugs is of no significance. When freezing due to permafrost growth starts, the repository is closed and saturated and the tunnel plugs have no performance requirement at this stage.

Handling in the safety assessment SR-Site

Process is neglected since there are no long-term performance requirements on the plugs.

5.2 Hydraulic processes

5.2.1 Water uptake and transport under unsaturated conditions

Overview/General description

The **hydro-mechanical evolution** of the plugs is as follows:

After installation, water will seek its way to the drainage material, mostly from the backfill that is not able to seal inflowing water, until the hydraulic gradients inside the tunnel has ceased. The water that flows into the drainage material will be drained from the top after filling up the drainage section. This drainage will continue until the plug functions mechanically, which takes a few months. During this time, water will not come in contact with the bentonite seal unless directly from inflow from the rock. There will thus be no or insignificant wetting of and swelling pressure in the bentonite seal until the drainage is closed. It should be noted that the water that drains out may contain eroding backfill material.

When the drainage has been closed, water will enter the bentonite seal and a successive wetting of the bentonite takes place and eventually a water pressure will build up and act on the plug. Although the plug is grouted, water may leak past the plug. This leakage will stop rather soon, since water has to pass either the bentonite seal or the backfill pellets before it enters the leaking fractures, and investigations have shown that bentonite in contact with leaking fractures will seal if the fractures are smaller than 100 μm /Sandén et al. 2008/.

With time, the bentonite seal will be saturated and exert full swelling pressure and water pressure on the plug. Due to the swelling pressure from both the backfill and the bentonite seal, the sand filter (drainage material) will be compressed and some of the swelling pressure on the concrete plug is lost.

The plug has fulfilled its purpose to prevent water flow and eroding bentonite out of the tunnel when full water pressure is reached outside the plug. When there is full water pressure on both sides of the plug, the plug will start its slow degrading process. When the mechanical function is lost, the swelling pressure inside the plug will affect the plug as listed below.

- A small axial displacement of the plug and compression of the crushed rock outside the plug will take place for the outer plugs, which are located between the transport tunnels and the crushed rock in the central area.
- The inner plugs between deposition tunnels and transport tunnels will have the same swelling pressure on each side after full water saturation and the resulting displacements will thus be small and only include compression of the plug parts, mainly the filter.
- The bentonite seal will swell into parts of the degraded plug and also into the open slot that exists in the roof of the crushed rock filling

Due to the friction in the bentonite and crushed rock there will be a remaining small axial density gradient in the backfill inside the plug, in the bentonite seal and in the crushed rock outside the plug.

A special case that may need some attention is if the crushed rock **outside** the plug is water saturated and exerts a hydraulic pressure on the plug before the backfill and bentonite seal become water saturated. Since the plug is not designed to withstand pressure from outside it may fail and water may thus flow into the backfill inside the tunnel. This case may not be a problem for the repository performance, but will be investigated.

The process “water uptake and transport under unsaturated conditions” treated in this section is only relevant for the bentonite seal, and the following description as well as the influence table refers to this part of the plug.

The process is described in detail in both the buffer and the backfill Sections (3.3.1 and 4.2.1) and will not be described here.

Dependencies between process and tunnel plug variables

Table 5-2 summarises how the process influences and is influenced by all tunnel plug and how these effects are treated in SR-Site. The table is relevant only for the bentonite seal in the plug.

Table 5-2 . Direct dependencies between the process “Water uptake and transport under unsaturated conditions” in the bentonite seal in the plug and the defined tunnel plug variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Plug geometry	Yes	Geometry included in the models	No	
Pore geometry	Yes. Via void ratio (density) and void geometry	Variable in the model	(Yes) If erosion takes place (secondary effect)	See erosion
Temperature	Yes. Indirect through water viscosity and hydrovariables in a temperature gradient	Negligible	Yes Wetting and drying affects thermal conductivity	Negligible
Water content	Yes. Via degree of saturation and retention properties	Variable in the model	Yes	Variable in the model
Gas content	Yes. Via the gas pressure and degree of saturation	Variable in the model	Yes	Variable in the model
Hydrovariables (pressure and flows)	Yes. Basic variables.	Variable in the model	Yes	Variable in the model
Stress state	Yes	Variable in the model	Yes	Variable in the model
Plug materials – composition and content	Yes. Hydraulic conductivity and retention curve etc.	Sensitivity analyses	(Yes). If erosion takes place (secondary effect)	See Section 5.2.4
Porewater composition	Yes	Controls some parameters in the model	Yes	See Section 5.4

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 tunnel, which distributes water from the fractures along the rock wall, the wetting will be faster and more even. This interaction is identical to the interaction with the backfill in the tunnels.

Interaction with the other parts within the plug: The bentonite seal in the plug has a wall of concrete beams on each side, which in turn are in contact with the drainage material and the concrete plug. The grain size distribution and compaction in the drainage material is designed such that the filter can collect and drain water so that the concrete plug will not be exposed to high water pressures until it has gained sufficient strength. It is designed and verified in accordance with conventional geotechnical procedures. When the drainage of the filter is closed a water pressure may build up and axial wetting may also take place.

Since the plug is demanded to be water tight also before the bentonite seal is water saturated, water flow and water pressure derived from the backfill inside the plug will be stopped and the leaking fractures sealed by the bentonite in the seal.

Model studies/experimental studies

All studies performed on wetting are done for the backfill and the buffer (see Sections 3.3.1 and 4.2.1).

Some tests have been performed to study the sealing ability of a pellets filling of unsaturated bentonite in contact with fractures of different widths. The results indicate that fractures with a width of 100 mm will be sealed /Sandén et al. 2008/.

Additional studies of the consequences on saturation of a high water flow and water pressure on the bentonite seal inside the plug before full swelling will be done /Åkesson et al. 2010a/.

Natural analogues/observations in nature

Wetting of bentonite in nature has not been studied and can probably not contribute to the knowledge.

Time perspective

Analyses made for the backfill and the buffer show that the time to full water saturation can vary a great deal, depending above all on the interaction with surrounding rock and the axial water transport in the tunnel. If conditions are wet with respect to 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 or more in the granitic rock types occurring in Sweden. Artificial wetting through the filter has been studied and show that the time to saturation may be reduced /Åkesson et al. 2010/.

Handling in the safety assessment SR-Site

All calculations done so far have concerned the buffer and backfill and the process is very similar for the bentonite seal in the plug. However, a hydro-mechanical sensitivity analyses is done in order to evaluate the concrete plug is affected by the swelling pressure.

The water saturation evolution of the bentonite seal as well as the sealing properties of the plug will be modelled and reported in the general THM modelling report /Åkesson et al. 2010a/.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

The general THM modelling report /Åkesson et al. 2010a/ will undergo a documented factual- and quality review.

Uncertainties

The uncertainties are the same as those reported for the corresponding buffer and backfill processes (see Sections 3.3.1 and 4.2.1).

5.2.2 Water transport under saturated conditions

Overview/General description

As described in section 5.2.1, the plug is required to seal for a short period only. The hydro-mechanical evolution of the plug is described in that section. After full water saturation and when the hydrostatic water pressure is reached, the plug has no sealing function and very little water will flow past the plug due to the low hydraulic gradient. The plug will thus be an integrated part of the backfill and will have one very tight section with the bentonite seal and two highly permeable sections (the filter and the concrete plug). However, the permeable sections are only local and will not influence the overall hydraulic behaviour of the tunnel backfill.

On these reasons, water transport under saturated conditions in the plugs will be handled very briefly. The process is already described for the buffer and tunnel backfill in Sections 3.3.2 and 4.2.2, respectively.

Dependencies between process and tunnel plug variables

Table 5-3 summarises how the process influences and is influenced by all variables of the plugs and how these effects are treated in SR-Site.

Table 5-3 . Direct dependencies between the process “Water transport under saturated conditions” and the defined tunnel plug variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Plug geometry	Yes	The process is neglected based on the discussion in this section	No	The process is neglected based on the discussion in this section
Pore geometry	Yes. void ratio (density) and void geometry	Negligible	(Yes) If erosion takes place (secondary effect)	See Section 5.2.4
Temperature	Yes. affects water viscosity	Negligible	No	
Water content	Indirect through pore geometry (density)		No	
Gas content	No, there is no gas phase in a saturated plug.		No	
Hydrovariables (pressure and flows)	Yes. Basic variables.	Negligible since very local influence	Yes	Assumed to be a local part of the tunnel with high hydraulic conductivity
Stress state	Yes	Negligible	Yes	Dimensioning. The plug must be able to withstand hydraulic water pressure.
Plug materials – composition and content	Yes. Hydraulic conductivity	Negligible since very local influence	(Yes). If erosion takes place (secondary effect)	Neglected, since extent is limited
Porewater composition	Yes through viscosity	Negligible	Yes, from degrading substances	Negligible

Boundary conditions

Only outer boundaries exist. There are three types of outer boundaries of the plug:

- The rock surface of the tunnel,
- The interface between the backfill and the drainage section,
- The interface between the outer backfill of crushed rock (or bentonite in some parts) and the concrete plug.

Model studies/experimental studies

Only studies of buffer and backfill material have been done and special studies of the plug function after saturation is not required.

Natural analogues/observations in nature

Not applicable

Time perspective

When full water saturation and hydrostatic pressure has been reached, which may take up to 100 years, the plug has no function. There may be a period after which full saturation in the plug and the bentonite seal has been reached when there is still a high hydraulic gradient across the plug due to possible very slow wetting inside the plug at dry tunnels. However, this situation is more favourable than if the plug and the bentonite seal are not saturated and will not be further dealt with.

Handling in the safety assessment SR-Site

Due to that there is no demand of the plug after saturation this process will not be handled in SR-Site in any other way than a discussion around a local part of the tunnel with higher hydraulic conductivity.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

No references required for this process.

Uncertainties

The average hydraulic conductivity of the plug after degradation is not known but a high pessimistic value may be used.

5.2.3 Gas transport/dissolution

Overview/General description

Gas processes in the plugs are only relevant for the saturation period and only for the bentonite part of the plug – this is described in Section 5.2.1

Handling in the safety assessment SR-Site

The process is treated as a part of the THM description of the plug, see Section 5.2.1.

5.2.4 Piping/erosion

Overview/General description

The process of erosion is described in the buffer chapter, Section 3.3.4. Since erosion is mainly a concern for the bentonite seal in the plug, the same description is valid here.

After full saturation and reestablishment of hydrostatic water pressure, the plug is not required to have any sealing function. Any consequences of erosion of the plug itself are thus not important. The plug and bentonite seal are instead required to stop eroding water from the tunnel to pass the plug during the saturation phase. The bentonite seal is expected to prevent leakage. If there are open fractures between the concrete and the rock, and water flows through these fractures due to malfunction of the bentonite seal when the plug is expected to seal, the function of the plug is not fulfilled. However, erosion will help to seal these fractures since the eroding material will get stuck and clog the fractures as shown in tests.

Erosion of the bentonite seal is thus not a problem but will instead stop flow past the plug.

Dependencies between process and tunnel plug variables

Table 5-4 summarises how the process influences and is influenced by all tunnel plug variables and how these effects are treated in SR-Site. The table is relevant only for the bentonite seal in the plug.

Boundary conditions

The piping and erosion that are mainly treated here only take place in the pellets-filled part between the clay blocks in the clay seal and the rock.

Table 5-4. Direct dependencies between the process “Piping/erosion” in the bentonite seal in the plug and the defined tunnel plug variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Plug geometry	Yes	No specific assessment of piping in the plug will be done	No	
Pore geometry	Yes, via density	Unimportant	(Yes)	Unimportant
Temperature	No		No	
Water content	Yes, via swelling pressure etc.	Unimportant	Yes	Unimportant
Gas content	Yes	Unimportant	Yes	Unimportant
Hydrovariables (pressure and flows)	Yes	No specific assessment of piping in the plug will be done	Yes	Sensitivity assessments for the hydraulic properties of the entire tunnel will be done
Stress state	Yes	No specific assessment of piping in the plug will be done	Yes	Via saturation rate (water content)
Plug materials – composition and content	Yes	No specific assessment of piping in the plug will be done	No	
Porewater composition	Yes	No specific assessment of piping in the plug will be done	No	

Model studies/experimental studies

The processes have been 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 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 built-up of water pressure in the fracture is fast.

Although the plug is grouted, it may leak water past the plug. This leakage will stop rather soon since water has to pass either the bentonite seal or the backfill pellets before it enters the leaking fractures, and investigations have shown that bentonite in contact with leaking fractures will seal if the fractures are smaller than 100 µm. The experiments are described in the chapter about unsaturated flow (Section 5.2.1).

At present, the processes are studied in the project *Backfilling and closure of the deep repository*.

Natural analogues/observations in nature

Not applicable for this process.

Time perspective

The piping and erosion only takes place before complete saturation and homogenisation. The high swelling pressure of the clay will ultimately always seal the piping channels, since the sum of the swelling pressure and the porewater pressure in the clay part of the plug will always be higher than the water pressure if the final average density of the clay is high enough.

The sealing expected to take place by the eroded bentonite will take place before full saturation is reached and thus only relevant for less than 100 years.

Handling in the safety assessment SR-Site

The process for the plug will not be separately handled in SR-Site. Possible erosion from the bentonite seal does not influence the overall safety since the seal has no function after full saturation of the surrounding tunnels and rooms. The consequences of an increased hydraulic conductivity in the entire tunnel are discussed in Sections 4.2.2 and 4.4.1.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

See the corresponding process in the buffer chapter, Section 3.3.4.

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 plug to handle the processes. The tests performed for the backfill project are expected to yield better understanding. Only the sealing ability of the eroded material is of interest. See also buffer Section 3.3.4.

5.3 Mechanical processes

5.3.1 Swelling/mass redistribution

The swelling process has been merged with other processes that cause mass redistribution within the plug, namely thermal expansion, creep and a number of interactions with the buffer, near field rock and the neighbouring backfill.

Overview/General description

The plug is a complex composite of different materials. A general description of the plug, its required function and the hydro-mechanical evolution are given in Section 2.4.1. The description shows that there are some mechanical processes that are important for the function. These are described in Section 5.2.1.

The mechanical processes associated with the bentonite seal in the plug are identical to those of the buffer and the backfill and are described in Sections 3.4.1 and 4.3.1, respectively.

Dependencies between process and tunnel plug variables

Table 5-5 summarises how the process influences and is influenced by all variables of the tunnel plug and how these effects are treated in SR-Site.

Boundary conditions

The plug has the rock, the inner backfill and the outer backfill material as boundaries. On the other hand the plug itself contains at least five parts that interact mechanically. Three walls of concrete beams are intended to separate the different parts of the plug from each other. The beams only have a mechanical function required for the installation period and will be design to come loose from the rock at very small axial pressure. This means that they will mechanically move as a passive boundary between the different parts of the plug.

Interaction backfill / drainage material

The backfill will during saturation increase its swelling pressure and compress the drainage material.

Interaction drainage material / bentonite seal

The bentonite seal will also increase its swelling pressure during saturation and compress the drainage material.

Table 5-5. Direct dependencies between the process “Swelling/mass redistribution” and the defined tunnel plug variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Plug geometry	Yes	Geometry included in the models	No	
Pore geometry	Yes. Via void ratio (density) and stress	Included in the models	Yes	Included in the models
Temperature	Yes. Thermal expansion	No, negligible	No	
Water content	Yes, the water content of the bentonite seal and in the sand filter.	Variable in the models	Yes	Variable in the models
Gas content	Yes. Degree of saturation and gas pressure	Included in the models	Yes	Included in the models
Hydrovariables (pressure and flows)	Yes. Basic variables.	Variable in the models	Yes	Variable in the models
Stress state	Yes	Variable in the models	Yes	Variable in the models
Plug materials – composition and content	Yes. Determines many parameters in the models	Sensitivity analyses	No	
Porewater composition	Yes. Influences many parameters in the models	Sensitivity analyses	No	

Interaction bentonite seal / concrete plug

The bentonite seal will increase its swelling pressure during saturation and stress the plug. In addition, there will be a hydraulic pressure on the concrete plug. The concrete plug is designed to withstand this pressure so it will only move slightly and improve the contact with the rock in the slot.

Interaction concrete plug / backfill outside the plug

If the backfill outside the plug consists of crushed rock, which will be the case for the plug facing the central area, there is no pressure on the plug from that side until a water pressure is built up. However, this interaction has two implications that must be considered:

1. If the water pressure outside the plug comes before swelling, (i.e. the central area is water filled before the backfill in the tunnel) and water pressure is derived inside the concrete plug there may be consequences for the plug since it is not designed to take such pressure. This implies that the concrete plug may break and that water may flow backwards through the plug. However, there are probably no negative consequences of this case, but this may need to be investigated.
2. After long time the concrete plug is degraded the bentonite from the bentonite seal and the backfill inside the plug may expand and penetrate into the possible open spaces in the plug and further on into the slot between the roof and the crushed rock in the backfill of the central area. In stagnant water, this is not expected to yield problems and can be estimated but if there is water movements in the slot there may be substantial erosion. This case may need to be investigated or prevented with an engineering solution.

Model studies/experimental studies

The mechanical processes relevant to the bentonite seal are the same as those reported for the buffer and backfill; see Sections 3.4.1 and 4.3.1, respectively. No other studies have been done so far but are planned.

The mechanical effect on the plug is handled by the design and related calculations provided in the Backfill production Report /SKB 2010e/.

Time perspective

The mechanical interaction is relevant during the entire lifetime of the repository. Although the plug has no function after about 100 years, the long-time effect of erosion of bentonite penetrating into the slot can continue if no other solution is invented.

Natural analogues/observations in nature

Not applicable.

Handling in the safety assessment SR-Site

The mechanical performance of the plug is discussed in the Backfill Production Report /SKB 2010e/

The water saturation evolution and the evolution of the stresses and displacements of the bentonite seal are modelled and reported in the general THM modelling report /Åkesson et al. 2010a/ as well as the swelling of the backfill and the bentonite seal following the disintegration of the plug.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

The general THM modelling report /Åkesson et al. 2010a/ and the Backfill Production Report /SKB 2010e/ will undergo a documented factual- and quality review.

Uncertainties

Uncertainties in mechanistic understanding

The mechanistic understanding of the mechanical processes is sufficient for the safety case.

Model simplification uncertainties in SR-Site

See above.

Input data and data uncertainties in SR-Site

The largest uncertainty is probably the fact that the design of the plug still is preliminary. A good modelling of the process can be done when a final design has been decided.

5.4 Chemical processes

5.4.1 Advection

Overview/general description

In this context advection refers to transport of any forms of additional matter, e.g. ions, molecules or colloids, with porewater flow. The transport direction is thereby principally from volumes of high water pressure to volumes of lower pressure. The advection is closely related to water flow in the tunnel plug, which is described in Section 5.2.2.

The maximum pressure gradients over the tunnel plug will occur during the installation period when one side of the plug will be pressurised by the hydrostatic pressure and the other side is kept drained. After closure, different inflow rates and volumes in the compartments may lead to a significant gradient. After full water saturation of the compartments, the pressure gradient will be induced by the regional pressure gradients, and comparatively much smaller. Additional causes of small pressure gradients may also be present by e.g. differences in salinity and temperature on the two sides of the plug.

Dependencies between process and tunnel plug variables

Table 5-6 summarises how the process influences and is influenced by all tunnel plug variables and how these effects are treated in SR-Site.

Table 5-6. Direct dependencies between the process “Advective transport of solutes” and the defined tunnel plug variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Concrete geometry	Yes, greatly by cavities and fracture	The process is neglected based on the discussion in section Water transport, Section 5.2.2	No, but indirectly through porewater composition and dissolution/precipitation	
Concrete pore geometry	Yes, dominating effect through hydraulic conductivity	Neglected	Yes, through dissolution/precipitation	Irrelevant since no performance is expected
Temperature	Yes, indirect through water viscosity	Neglected	No	
Water content	Yes, by definition	Neglected	No	
Gas content	Yes, through water content	Neglected, will always reduce the process	Yes, dissolution/release of gas	Irrelevant since no performance is expected
Hydrovariables (pressure and flow)	Yes, by definition	Neglected	Yes, by definition	Irrelevant since no performance is expected
Stress state	Yes, hydraulic conductivity is related to swelling pressure in the bentonite. Through fracture aperture in the concrete	Neglected	Yes, minor through osmotic effects and precipitation/dissolution	Irrelevant since no performance is expected
Concrete composition	Yes, through porosity/hydraulic conductivity	Neglected	Yes, through dissolution/precipitation	Irrelevant since no performance is expected
Concrete porewater composition	Yes, by definition	Neglected	Yes, by definitions	Irrelevant since no performance is expected

Boundary conditions

The external boundary condition for this process is the hydraulic pressure gradient and the concentration gradients for species across the tunnel plug system component.

Model studies/experimental studies

Similar types of plugs are present in the Äspö HRL, and have been examined with respect to water flow. A vast knowledge concerning concrete construction in general is present and may to a large extent be used for the specific tunnel plug repository compartment.

Natural analogues/observations in nature

Nothing relevant.

Time perspective

Advective flow transport in conjunction with water saturation takes place on a timescale of up to hundreds of years. After full saturation of the tunnel system, the advective transport is expected to be low due to the minor pressure gradients. However, the function of the plug will eventually be lost due to degradation of the concrete.

Handling in the safety assessment SR-Site

Since there are no requirements on stability of the plug after saturation of the repository, this process will not be handled in SR-Site in any other way than as a discussion of the implications of a local part of the tunnel with higher hydraulic conductivity.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

No references required for this process.

Uncertainties

The average hydraulic conductivity of the plug after degradation is not known but a high pessimistic value may be used

5.4.2 Diffusive transport of species

Overview/general description

An overview of diffusion processes and phenomena relevant for bentonite and concrete are given in Sections 3.5.3 and 8.4.2, respectively. These considerations also apply to the concrete- and bentonite-parts of the tunnel plug. /Luna et al. 2006/ conclude that the main diffusion parameters (including porosity) will not be significantly affected by an alkaline plume.

Handling in the safety assessment SR-Site

These system components are not included in the radionuclide transport calculations. Diffusion is neglected, since advection will dominate in a degraded plug.

5.4.3 Sorption (including exchange of major ions)

Overview/general description

Sorption processes relevant for the concrete part of the plug are the same as those for the concrete bottom plate described in Section 8.4.3, and for the bentonite seal, the processes are the same as those for the buffer described in Section 3.5.5. Concrete-bentonite interaction occurring at the interface of the two parts of the tunnel plugs may lead to changes in the mineralogy of the respective materials, which will also influence sorption.

Handling in the safety assessment SR-Site

Sorption of radionuclides in tunnel plugs is neglected in SR-Site.

Uncertainties

Uncertainties in mechanistic understanding

Uncertainties in mechanistic understanding are discussed in Section 3.5.5 for sorption on bentonite, and briefly in Section 8.4.3 for sorption/uptake on concrete.

Model simplification uncertainty in SR-Site

Not applicable since sorption in tunnel plugs is neglected.

Input data and data uncertainties in SR-Site

Not applicable since sorption in tunnel plugs is neglected.

5.4.4 Alteration of concrete

Overview/general description

The cement-water mixture is transformed into hardened cement paste, with main binding phases comprising calcium silicate hydrates (CSH) and calcium hydroxide (CH). In addition, two other major hydration products are produced from reactions involving the aluminate, alumino-ferrite, and calcium sulphate, known as AFt and AFm, which are complex calcium ferri-aluminates.

Hardened cement paste is a porous material, due to the large water/cement ratio of the original cement grouting. The interstitial solution of an ordinary Portland-cement-based paste will reach chemical equilibrium with the cement constituents, resulting in a hyperalkaline porewater (pH around 13) with large concentrations of alkaline Na^+ , K^+ , OH^- and Ca^{2+} ions. In the future Swedish spent fuel repository, it is planned to use a “low-pH” cement, although the actual recipe, Backfill Production Report /SKB 2010e/, will probably be optimised before the repository construction and during the relatively long period of repository operation. The concept behind the elaboration of such low-pH grout lies in the substitution of cement by considerably large amounts of silica fume. One of the main advantages of the addition of silica fume into the mixture of grout consists of a remarkable decrease of the volume fraction of the highly soluble portlandite ($\text{Ca}(\text{OH})_2$). It also contributes to reduce the content of aluminum compounds and to lower the pH of the pore solution. Indeed, the porewater pH in equilibrium with low-pH cement constituents is estimated to be around 11 or lower. This particular feature has beneficial effects on long-term safety because the porewater of the material is much less reactive with the bentonite clay that surrounds the copper canisters in the repository. Yet, the contact of this alkaline cement porewater with dilute groundwater (pH lower than 9) creates large concentration gradients which induce diffusive mass transport (of mainly Ca^{2+} and OH^- ions) outwards from the porous cement paste. Renewal of the external groundwater by advection will drive away the cement porewater components and accelerate the diffusion of ions and the degradation of cement component. The alkaline cement porewater will react with fracture filling and rock minerals through a complex set of reactions that finally neutralise the alkalinity and produce calcium silicate hydrates, see for example /Hoch et al. 2004, Wan et al. 2004/.

The durability of cement paste is affected by the decalcification process, since calcium is the main component of cement hydrates. The continuous outwards diffusion of Ca^{2+} alters the original chemical equilibrium, which induces dissolution of calcium compounds as the natural tendency is to restore chemical equilibrium. The dissolution of highly soluble calcium hydroxide (portlandite) and CSH phases leads to an increase in the porosity of the cement paste, which at the same time enhances the diffusion rate. Low-pH cements have negligible quantities of portlandite and larger amounts of CSH phases than ordinary Portland cements. CSH solubility is complex due to its amorphous to semi-crystalline structure, which might be described in terms of a mixture of tobermorite-like phases with others of jennite-like structure /Taylor 1986/. Successive investigations have shown that CSH have a large variability in their composition, nanostructure and morphology /Richardson 2004/. Perhaps the most relevant features of CSH solubility concern their conditions of formation /Flint and Wells 1934, Roller and Ervin 1940, Taylor 1950, Kalousek 1952, Greenberg and Chang 1965, Fujii and Kondo 1981, Barret et al. 1983, Brown et al. 1984, Grutzeck et al. 1989/. Recent studies /Chen et al. 2004/ suggest that CSH solids are present under different metastable phases which are susceptible to transform (recrystallise) into one another in the long term.

Simultaneously with the dissolution of calcium silicate hydrates, the rest of the mineral phases are also involved in the cement leaching phenomena. AFm dissolution releases $\text{Al}(\text{OH})_4^-$ which will also out-diffuse and could induce precipitation of either secondary AFm or ettringite (in the presence of sulphates), whose large molar volume and crystalline morphology may close off the porous structure and reduce the mechanical strength of the cement by producing micro-cracks /Lagerblad 2001/. In the case of an external groundwater containing carbon dioxide, precipitation of calcite might be expected, which was found to reduce the degradation rate by sealing the pore network on the exposed surface of cement paste /Pfungsten 2001/. Brucite may also be prone to precipitate at the cement-groundwater interface, due to the lower pH environment /Lagerblad 2001/.

The chemical composition of groundwater or backfill porewater affects the rate of concrete plug degradation. Laboratory experiments have shown that the degradation depth is highly dependent on the carbonate concentration of the external solution. A study by /Moranville et al. 2004/ showed that leaching depth decreases by a factor of 5 when the external water is in equilibrium with atmospheric

CO₂, due to the sealing produced by calcite precipitation at the cement-water interface. An external groundwater containing dissolved sulphate could also have a large impact on the longevity of concrete material /Höglund 2001/ due to ettringite precipitation. The reason is that ettringite has the ability to bind crystal (“adsorbed”) water, resulting in a large molar volume of this mineral phase, which results in cracking and mechanical deterioration of the cement paste. Chloride concentration of the groundwater can also affect the long-term behaviour of the cement paste due to the precipitation of Friedel salts (i.e. aluminium and calcium chlorides).

Dependencies between process and tunnel plug variables

Table 5-7 shows how the process influences and is influenced by all tunnel plug variables.

Plug geometry: The geometry of the plug affects the process by considering the total mass of concrete and the reactive phases it contains. Therefore, the total pool of these mineral phases will affect the geochemical evolution of the system.

Pore geometry: The solid-to-liquid ratio will affect the degradation of concrete, at higher ratios the degradation will be slower, as a minor mass of minerals dissolved is needed to attain saturation. On the other hand, the dissolution – precipitation of cement mineral phases can modify the pore geometry and the total porosity of the system, and thus, modifying the degradation rate of concrete.

Temperature: Thermodynamic constants of chemical reactions are highly dependent of the temperature. However, temperatures in concrete plug are not expected to vary significantly, and therefore, minimal effects on the geochemical processes are foreseen.

Water content: This variable will affect the dissolution of cement phases as reactions can only take place in wetted surfaces. However, the process only considers full water saturation, as minimal changes are expected to occur until that time.

Table 5-7. Direct dependencies between the process “Alteration of concrete” and the defined tunnel plug variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Plug geometry	Yes	Plug mass considered	The degradation will reduce the mass	Plug mass considered
Pore geometry	Yes	The solid-to-liquid ratio is considered.	Yes. Dissolution – precipitation of solid phases can modify the porosity of the system.	Porosity changes due to dissolution – precipitation reactions is considered.
Temperature	Yes, temperature effect on thermodynamic constants.	Constant temperature assumed	No	
Water content	Yes, Could affect concentrations	Saturated conditions assumed	No	
Gas content	No		No	
Hydrovariables (pressure and flows)	Yes. Effect on reaction rates and transport of chemical components	Included in mass balance	No	
Stress state	No		No	
Plug materials – composition and content	Yes, reactivity with minerals. Cement mineralogy	Included in modelling	Yes, modification of mineral composition. Concrete degradation	Included in modelling
Porewater composition	Yes, Affecting reactivity of system components	Included in modelling	Yes, reaction with minerals results in changes in porewater composition	Included in modelling

Gas content: Gases can form or dissolve through chemical reactions, although their partial pressures are considered in the models, it is not expected that gases can form in the concrete plug.

Hydrovariables (pressure and flows): Transport of water and solutes is a very important variable on the degradation rate of concrete. The faster the solutes are transported away from the system, the faster the dissolution rates occurs, as the saturation state of those minerals being dissolved are maintained at low values. For the same reason, the precipitation of secondary phases will be inhibited, as the concentrations in porewater won't increase enough to reach saturation. However, if transport of solutes occurs at a slow rate, then dissolution of cement phases will occur at a slower rate, but precipitation of secondary phases is more likely to occur.

Stress state: This variable has no effect on the alteration of concrete process.

Plug materials – composition and content: This is one of the most relevant variables influencing this process. The type and amount of minerals is essential to determine how their dissolution – precipitation behaviour will affect the chemical evolution of the system, modifying both the porewater composition and the minerals present in the system (i.e. newly precipitated minerals and amount of existing minerals).

Porewater composition: The porewater composition will determine which of the minerals in the system will dissolve or precipitate, and thus the dissolution – precipitation of these minerals will modify the chemical composition of porewater.

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 solutes transport between the concrete plug, the backfill and the groundwater as adjacent system components, i.e. the boundary conditions of the processes diffusion and advection.

Model studies/experimental studies

A large amount of research has been reported in the scientific literature involving accelerated laboratory leaching tests, among the most recent papers are those of /Faucon et al. 1998, Carde et al. 1996, Saito and Deguchi 2000, Catinaud et al. 2000, Moranville et al. 2004/. Experimental evidence has also been reported on long-term leaching through the analysis of old, man-made, cementitious structures /Álvarez et al. 2000, Lagerblad 2001/.

From the modelling standpoint, works focused on the evaluation of the long-term deterioration of low-pH cement are still on an early stage of development since, as noted by /Savage and Benbow 2007/ “not all cement models are applicable to modelling low-pH systems”.

As /Benbow et al. 2007/ point out, modelling of cement degradation is a complex task in view of the long-term pH buffer is controlled by the incongruent dissolution behaviour of the CSH gel. In their report, an intercomparison is performed between three different models of CSH, namely the ones developed by /Börjesson et al. 1997/, /Walker 2003/ and /Sugiyama and Fujita 2005/. Both /Börjesson et al. 1997/ and /Walker 2003/ focus their approach to modelling solid solutions by providing a method of determining the solid phase activity coefficients based on the calculation of the excess energy of the solid solution as a function of its composition. The expression that relates the excess energy and the composition of the solid solution is of Margules type (i.e. the excess energy is expressed as a power series of mol fractions), under the form of the so-called Guggenheim mixing model. Their approaches, however, differ in the method applied calculating the Guggenheim parameters. On the other hand, /Sugiyama and Fujita 2005/ base their approach on the “conditional equilibrium constant”, but it can be related back to determining the solid phase activity coefficients. One additional difference between the models of /Börjesson et al. 1997/ and /Walker 2003/ with respect to the one developed by /Sugiyama and Fujita 2005/ consists of the selection of the end-members of the binary solid solution: the former consider portlandite ($\text{Ca}(\text{OH})_2$) and a CSH gel, it being expressed by an empirical formula (CaH_2SiO_4) representing the simplest stoichiometry of a CSH gel in terms of its component oxides; in the latter's model, the end-members are taken to be $\text{Ca}(\text{OH})_2$ and $\text{SiO}_2(\text{s})$.

Whereas results of the intercomparison have shown that the three models are generally in agreement with the behaviour of the cement, the different choice of end-members may make the Sugiyama and Fujita model more advantageous regarding the modelling of low-pH cements, since the lower values of the spectrum of Ca/Si ratios can then be contemplated.

Recent models of cement degradation have also addressed the task of considering the effects of evolution of physical properties (i.e. porosity, diffusivity) on the behaviour of the leaching process. Some of them on the basis of fitting curves derived from experimental data /Yokozeki et al. 2004/ and some others on either “pure” random models /Bentz and Garboczi 1992/ or “hybrid” models, where randomness is constrained by appropriate user-defined probability distributions /Marchand et al. 2001/. A pure mechanistic approach for cement degradation modelling requires the coupling of multi-component solute diffusion and chemical reactions taking place in the system. Dimensionless analyses of diffusion and reaction rates demonstrate the adequacy of a local equilibrium assumption for coupled reactive transport modelling of cement leaching /Barbarulo et al. 2000/. By this approach, a mixed non-linear set of equations can be solved numerically. The domain of the problem could be represented either as a homogeneous medium, obtained by averaging the variables of interest over a representative elementary volume, or a pore structure modelled on the basis of microstructural information, such as that provided by mercury intrusion porosimetry, or on the reconstruction of the microstructure by means of random models /Bentz 1999/. The latter was recently addressed in /Moranville et al. 2004/.

A relevant decision to be taken in the reactive transport-based models of cement degradation arises from the selection of the geochemical processes to be included. The inclusion of K^+ , Na^+ , Mg^{2+} , Ca^{2+} , SO_4^{2-} , OH^- , $Al(OH)_4^-$ and Cl^- , is claimed in /Maltais et al. 2004/ to be sufficient to describe most degradation processes, although other sets of chemical components have also been proposed, e.g. in /Höglund 2001/.

Natural analogues/observations in nature

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

Time perspective

Since cement leaching is mainly a coupled diffusion-reaction phenomenon, the time needed for complete degradation of concrete plugs will be highly dependent on the relative surface area of the concrete where diffusion exchange with backfill porewater can take place. This parameter will be related to the thickness of the plug. However, the porosity and permeability increase due to concrete degradation is not always taken into account which could lead to an overestimate of the calculated degradation times.

Handling in the safety assessment SR-Site

The cement plug durability is important as its degradation can result in an increased pH in the near field in the repository. The rate of degradation will impact the geochemical conditions in the contact area with the backfill and potentially also further away from the plug. Therefore, the cement plug durability has to be evaluated by long term reactive transport modelling, accounting for the coupling between dissolution/precipitation of minerals and porosity/diffusivity/hydraulic conductivity changes.

The models evaluate quantitatively the long term durability of cementitious components of the repository, including the time evolution of the main physical and chemical properties, the time evolution of the hydrochemical conditions close to the cementitious components as a result of the alkaline perturbation produced by cement leaching, and the hydrogeochemical effects produced by the alkaline perturbation on the adjacent barriers.

Handling boundary conditions:

The degradation of cementitious components will be highly dependent on the external boundary conditions. On one hand, the rate of external groundwater renewal and the chemistry composition of the external groundwater have a strong influence on the out diffusion of ions from the cement paste: a renewal of the external groundwater by advection would accelerate the degradation of cement. On the other hand, the chemistry of the external groundwater will also influence the processes. For example, high carbonate concentrations in the external groundwater would probably produce calcite precipitation and/or the precipitation of other secondary minerals, which may reduce the porosity and therefore the cement degradation rate.

Handling influences between variables and process:

Cement degradation phenomena have a strong coupling between physical and chemical processes. Then, solute transport and geochemical reactions should be coupled in the models to account for relevant processes such as dissolution/precipitation of CSH gels and porosity changes due to mineral dissolution and precipitation. At the same time, changes in porosity are coupled with solute diffusion and water flow, so numerical models should account for these fundamental relations.

Handling coupling to other processes:

Cement degradation will produce an alkaline perturbation and a leachate plume that could reach the buffer, backfill and geosphere. The performance requirement for the buffer is currently a $\text{pH} < 11$. The purpose of the handling of this process is to demonstrate that this requirement is met. The interaction of the hyperalkaline plume with the external groundwater could trigger mineral dissolution/precipitation processes that could influence the groundwater flow and solute transport properties of the buffer, backfill and geosphere. Coupled reactive transport models should account for these couplings in order to evaluate the magnitude these effects.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

The main part of the references cited is peer reviewed papers.

Uncertainties**Uncertainties in mechanistic understanding**

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

Model simplification uncertainty in SR-Site

The calculations to evaluate the degradation of the concrete plug can be made using a simplified 2D geometry, where the plug is sandwiched between two sections of bentonite backfill. Furthermore, the solid phases considered is a simplification of the CSH phases that really precipitate. The implications of this will be discussed in the modelling report /Arcos et al. 2010/.

Input data and data uncertainty in SR-Site

The main uncertainties concern the composition of the concrete plug and the thermodynamic stability of calcium-silicate-hydrates. The implications of this will be discussed in the modelling report /Arcos et al. 2010/.

5.4.5 Aqueous speciation and reactions

Overview/general description

This process is in general identical with the corresponding process in the buffer (Section 3.5.7).

Handling in the safety assessment SR-Site

The process is included in a separate modelling task of the plug (concrete part) degradation. This is further described in Section 5.4.4.

5.4.6 Osmosis

Overview/general description

Flow of a solvent into a solution through a semipermeable membrane is termed osmosis if the driving force is differences in concentration. The concrete may serve as a semipermeable membrane and osmotic flow may take place in the system component.

Handling in the safety assessment SR-Site

The magnitude and especially the lack of significant osmotic flow in the tunnel plug make this process less important and will not be considered in SR-Site.

5.4.7 Montmorillonite transformation

Overview/general description

This process is in general identical with the corresponding process in the buffer (3.5.9) for the bentonite part of the plug.

Handling in the safety assessment SR-Site

The process is neglected since no long term performance is expected from the bentonite part in the tunnel plug component.

5.4.8 Montmorillonite colloid release

Overview/general description

This process is in general identical with the corresponding process in the buffer (3.5.11) for the bentonite part of the plug.

Handling in the safety assessment SR-Site

The process is neglected since no long term performance is expected from the bentonite part in the tunnel plug component.

5.4.9 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 /Madigan et al. 2008/.

Plastisiers that will be added to the concrete will contain organic polymers of varying compositions, e.g. polycarboxylate polymers. The amounts to be used will be significant. The amount of plastisiers will be 6-7 kg /m³ concrete (Table 2-10). Plastisiers introduce a significant uncertainty, because their composition and solubility, and thereby their availability to microbes, are not well known. In cases where a grouting activity fails and the grout do not solidify properly; large amount of organic carbon will be available for microbial growth. Such growth can occur in the grouted aquifers and in the central area, ramp and shaft on places where groundwater from grouted sites seep through the tunnel walls.

Dependencies between the process and the tunnel plug variables

Table 5-8 shows how the process influences and is influenced by all tunnel plug variables.

There are two main influences from the structural material variable on microbial processes.

1. Microbial sulphate reduction during microbial growth on plastisiers will result in sulphide. The sulphide may accumulate as iron sulphide inside the plugs. During the open phase, oxygen will oxidise the sulphide and sulphuric acid can form. Local acid attacks on the concrete may occur. This effect will diminish after backfilling on both sides of the plug, when oxygen is consumed, but it may introduce a problem during the open phase.
2. Excess amounts of organic material in aquifers will trigger growth of opportunistic microorganisms that will increase in numbers. Several groundwater microorganisms produce complexing agents that very efficiently mobilise trace elements, including many radionuclides /Kalinowski et al. 2004, 2006, Johnsson et al. 2006, Essén et al. 2007, Moll et al. 2008/. Given the large amount of added organic carbon where grouting have been performed, it is possible that the microbial production of complexing agents will be significant which may notably reduce the retardation effects accounted for by the rock and the rock matrix.

Table 5-8. Direct dependencies between the process “Microbial processes” and the defined tunnel plug variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Plug geometry	No		No	
Pore geometry	No		Growth of microbes generate biomass that may clog pores	This effect is not considered in SR-Site
Temperature	Yes, microbial activity increases with temperature	This effect is not considered in SR-Site	No	
Water content	Yes, availability of water	Saturated conditions assumed	No	
Gas content	Indirectly through water content		No	
Hydrovariables (pressure and flows)	Yes, water is needed for growth of microbes and growth on hydrogen and methane is possible. Pressure is not important	This effect is not considered in SR-Site	Yes, microbes may form methane and hydrogen	This effect is not considered in SR-Site
Stress state	No		No	
Plug materials – composition and content	Yes, the content of organic carbon and microbes in different backfill clays varies	This effect is not considered in SR-Site	No	
Porewater composition	Yes, microbes are sensitive to the geochemical situation, and may utilise pore-water components for growth	This effect is not considered in SR-Site	Yes, microbial activity may change the composition, e.g. by consumption of methane, sulphate and organic carbon and production of sulphide and carbon dioxide.	This effect is not considered in SR-Site

Boundary conditions

The access to organic material, as organic additions to concrete, hydrogen from anaerobic corrosion of iron, organic material from other material that cannot be stripped or cleaned out and methane and electron acceptors from the geosphere will set the limits for the microbial processes in the plug. Given the large amount of plasticiser that will be added, access to organic carbon can be assumed for a long time.

Model studies/experimental studies

None.

Natural analogues/observations in nature

No relevant natural analogues or observations have been identified.

Time perspective

Microbial processes will start when water becomes available. The process rates will be largest in areas where organic carbon and hydrogen are available. Elevated microbial process rates, compared to the geosphere, will continue until all sources for growth have been consumed.

Handling in the safety assessment SR-Site

Mass balance calculations are 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.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

All the references in this section are from peer reviewed scientific journals. However, the most recent ones may be in the progress of being published. See also the same topic in Section 4.4.10.

Uncertainties

Uncertainties in mechanistic understanding

The knowledge about microbial processes in the plugs is not yet well supported by experimental data. Rather, the processes are inferred from research on microbial processes in the geosphere and in buffer material.

Model simplification uncertainties in SR-Site

The effects of microbial reactions are maximised since a mass-balance expression is used.

Input data and data uncertainties in SR-Site

The amount and availability of organic materials and metals in the plugs will determine the extent of microbial reactions. The data can be found in the Backfill Production Report /SKB 2010e/.

5.5 Radionuclide transport processes

5.5.1 Speciation of radionuclides

Overview/general description

See corresponding process description for the buffer, Section 3.6.1.

Handling in the safety assessment SR-Site

This process is indirectly handled through the selection of parameters for radionuclide transport in the backfill. In general, the handling of the process is the same as for the corresponding process in the buffer (see Section 3.6.1).

5.5.2 Transport of radionuclides in the water phase

Overview/general description

The plug covers a limited volume with tunnel backfill on each side (except the plugs facing the central area). The hydraulic conductivity of a degraded plug may be high and transport of dissolved species may be rapid, but since the geometry is restricted, the plug will not affect the overall transport pattern in the repository.

Handling in the safety assessment SR-Site

The plug is considered to be a part of the tunnel backfill in the radionuclide transport calculations. No specific considerations are done for the plug.

5.5.3 Transport of radionuclides in a gas phase

Overview/general description

The permeability for gas in the degraded tunnel plug may be high and they could potentially act as sink for a gas phase that is transported away from a defect canister. This could delay the release of radioactive gases from the repository.

Handling in the safety assessment SR-Site

The delay of a gaseous release of radionuclides is neglected in SR-Site. The overall process is treated according to Section 3.6.3.

6 Processes in the central area

6.1 Thermal processes

6.1.1 Heat transport

Overview/general description

The thermal conductivity of the repository host rock is in the range 2.0 – 4.0 W/(m·K) /Back et al. 2007, Sundberg et al. 2008/. The thermal conductivity of the crushed rock filling out shafts and ramps in the central area is significantly lower, although there are no parameter values available. In addition, the volume fraction of the central area or, more generally, of the rock between the deposition areas that is occupied by backfilled excavations is very small. These facts together mean that the thermal conditions in backfilled shafts and ramps are controlled and dominated by the temperature evolution of the surrounding rock, and that details in the description of the heat transport within the crushed rock backfill are unimportant.

The temperature increase in rock volumes between the deposition areas will be modest, at most c. 20-25°C a few hundred years after closure. Thermal gradients will be modest too: 5-10°C/100 m vertically in rock between deposition areas separated by 70 m, which would be representative for the location of the central area (Figure 6-1) /Hökmark et al. 2009/. The low temperatures and the small gradients mean that evaporation and vapour diffusion cannot contribute to the heat transport and that the influence of the heat transport on all variables other than the temperature are vanishingly small.

Dependencies between process and central area variables

Table 6-1 summarises how the process influences and is influenced by all crushed rock variables and how these effects are treated in SR-Site.

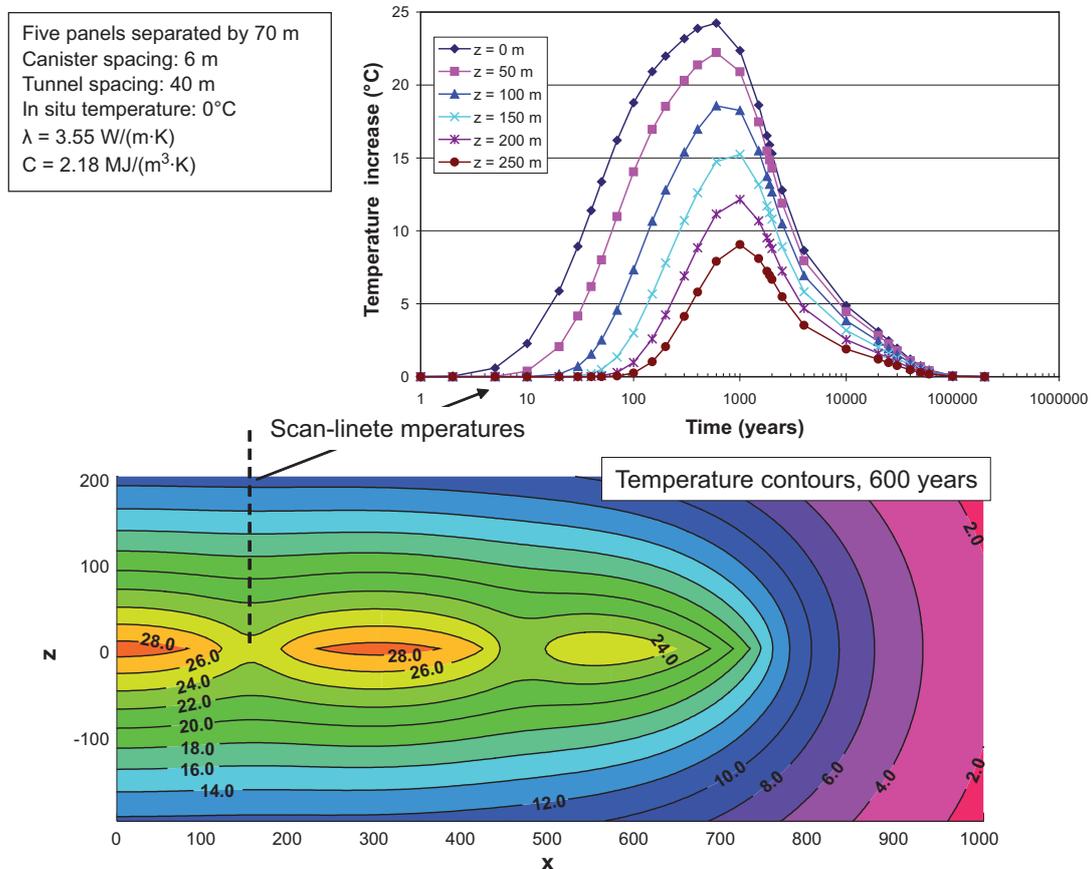


Figure 6-1. Example of contours of temperature increase (lower) and temperature increases on vertical scan-lines between deposition areas (upper). Results obtained using the method described in /Hökmark et al. 2009/.

Table 6-1. Direct dependencies between the process “Heat transport” and the defined central area variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Central area geometry	No		No	
Central area pore geometry	Yes. Affects thermal conductivity	Not specifically addressed since consequences are insignificant	No, but indirectly via temperature and thermal strain	
Temperature	Yes Rock heat transport is slightly temperature dependent.	Not specifically addressed Effect is very small for the modest temperature increase in the central area.	Yes. By definition	Ignored, since temperature increase in the central area is small and of no consequence
Water content	Yes	Not specifically addressed since consequences are insignificant	No	
Gas content	No, but indirectly through water content	-	No	
Hydrovariables (pressure and flows)	No		No, but indirectly via temperature	
Stress state	No		No, but indirectly via temperature and thermal strain	
Central area materials – composition and content	Yes	Not specifically addressed since consequences are insignificant	No	
Central area porewater composition	No		No	
Structural and stray materials	No		No	

Central area geometry: The geometry of the crushed rock filling out shafts and ramps is given by the shape of the excavations. This cannot be expected to change in a way that can affect the heat transport in the crushed rock. There will always be sufficient backfill/rock contact to ensure that the rock and the crushed rock are in thermal equilibrium.

Central area pore geometry: The crushed rock thermal conductivity varies with the void ratio, as for all porous materials and similar to the way it varies with the void ratio of the backfill in the deposition tunnels. The small thermal expansion of the solid particles will affect the void ratio very insignificantly.

Temperature: Heat transport influences the temperature by definition. There is a small temperature dependence in the heat transport properties of rock and crushed rock. For the modest temperature increase in the central area this is of no importance.

Water content: The heat transport will not affect the water content. The conductivity-saturation relations that apply for the buffer and the deposition tunnel backfill are in principle valid also for the crushed rock in the excavations in the central area. Since the thermal evolution in the central area is practically independent of the heat transport in the excavations, this is of no importance.

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, i.e. they are of no importance.

Hydro variables: The heat transport in the excavations does not control the temperature and consequently none of the hydro variables. Water flow can contribute to the heat transport, but high flow rates are required.

Stress state: Heat transport does not change the stresses. The stress state does not have any practically influence on the heat transport, although the crushed rock thermal conductivity may increase marginally when the stress increases. The effect is, however, too small and uncertain to be credited /Börgesson et al. 1994/.

Crushed rock composition: The composition of the backfill will influence the thermal conductivity. Some minerals have higher conductivities than others.

Crushed rock porewater composition: No influences.

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 peripheries of the excavated tunnels, intersections with other tunnels, tunnel faces and sealing tunnel plugs are the boundaries of the crushed rock. The boundary conditions of the process are the temperatures at these boundaries. 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 deposition areas. 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 central area. 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 the thermal evolution of the repository rock mass in general. Predictions of the temperature evolution have, for instance, been done analytically /Claesson and Probert 1996, Hökmark and Fälth 2003, Hedin 2004/ and numerically /Thunvik and Braester 1991, Ageskog and Jansson 1999, Hökmark et al. 2007/.

Natural analogues/observations in nature

Not applicable.

Time perspective

The duration of the thermal pulse generated by the decaying fuel is a few thousand years. The general statements made for the thermal pulse hold true also during following phases, i.e. heat transport in the excavations in the central area 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-Site

There is no specific handling of heat transport in the central area during the thermal phase since the temperature in the central area is not directly related to safety. Results from thermal analyses of the repository rock mass give sufficient information on the temperature in central area.

For permafrost and glacial conditions, the minimum temperature of the crushed rock may be of concern, see further Section 6.1.2. For these conditions, as well as for the conditions during the temperate period, the backfill temperature can be taken to be equal to that of the host rock. See further the SR-Site Geosphere process report /SKB 2010i/ for the treatment of rock temperatures for these conditions.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

Because of the small thermal gradients and the relatively low temperatures in the central area, there is no specific handling of the heat transport process. These statements are supported by results obtained using calculation schemes described in /Claesson and Probert 1996/. While this particular report is not peer- or factual reviewed, the calculation scheme has been repeatedly applied in peer reviewed papers /Hökmark and Claesson 2005/ and in reports that have undergone (/Hökmark and Fälth 2003/) or will undergo (/Hökmark et al. 2009/) a documented factual and quality review.

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 (should the process be modelled) the heat transport is expediently described as pure conduction with a saturation-dependent or fixed conductivity.

Model simplification uncertainties in SR-Site

Not relevant since the process is not modelled.

Input data and data uncertainties in SR-Site

Not relevant since the process is not modelled.

6.1.2 Freezing

Overview/general description

During periods of cold climate it cannot be excluded that the temperature in the central area will drop to values below 0°C /SKB 2010h/. This means that the water in the crushed rock backfill may freeze. This will affect the hydraulic and mechanical properties of the material.

The hydraulic conductivity of the crushed rock will be very much dependent on the grain size distribution, but is estimated to be in the range 10^{-6} – 10^{-7} m/s (see Section 6.2.1).

It is known that changes in hydraulic conductivity may take place in granular material due to freezing and subsequent thaw.

Largest changes in hydraulic conductivity are found if clay particles are present and fill the voids between the bigger particles. During the freeze/thaw process the fine grained fractions, filling the voids, will consolidate due to the freezing process. The coarser particles will create a stable structure controlling the compressibility and therefore no change in overall void ratio occur, but the clay particles will consolidate to a denser structure and consequently, the void space is filled with less, but denser, clay aggregates. The hydraulic conductivity will therefore increase due to freeze/thaw. This process only takes place if the amount of clay is in the order of approximately 10% or more. If the clay content is less, the changes in hydraulic conductivity will be very small, if any. In a coarse grained material, like the material used in the ramp and shafts, the created voids and cracks will be closed and sealed by relocation of small particles. /Viklander 1997/ states that a type of self-healing takes place during thaw. The conclusion and observations are supported by results presented by /White and Williams 1994/.

The overburden, or mean stress level, has impact on the changes in hydraulic conductivity due to freezing and thawing. For high stress levels, changes in hydraulic conductivity are relatively smaller than for lower, see e.g. /Benson and Othman 1993/. The stress level which is needed to keep the changes of hydraulic conductivity unchanged after freeze/thaw varies with the grain size distribution of the material. Highest stress levels are needed for the finest soils. For mean stress levels higher than 200 kPa, no changes in hydraulic conductivity have been reported due to freeze/thaw. For coarse grained material, 50-100 kPa is enough to close openings and fissures created by freeze/thaw /Viklander 1997/.

Particle migration and particle sorting are processes taking place in soils subjected to freezing and thawing. According to /Corte 1963/, coarse particles move towards colder parts where they are accumulated. Coarse particles (> 1 mm) need a low freezing rate to be moved. In laboratory tests, these phenomena are not found very often and /Corte 1963/ concludes that as the phenomena are easily observed in permafrost areas it indicates that a relatively great number of freeze/thaw cycles are needed to initiate the phenomena. /Corte 1963/ indicates that several hundreds of cycles might be needed in order to have the migration and sorting phenomena in a well graded moraine.

The phenomena with stone heave are related to the migration and sorting phenomena in a moraine subjected to cycles of freeze/thaw. Coarse particles and stones are lifted when embedded in a frost heaving soil. /Viklander 1997/ concludes that stone heave is restricted to approximately 5 mm/cycle. If the material in the central area volume is subjected to freezing conditions more than 1,000 times, this will imply that coarse material will be relocated to the top of the volume while more fine grained material will be found at lower levels of the tunnel. The mass of fill material in the volume stays constant, and therefore this will not have a great impact of the overall hydraulic conductivity even though there will be a redistribution and sorting of the particles.

Dependencies between process and central area variables

Table 6-2 summarises how the process influences and is influenced by all crushed rock variables and how these effects are treated in SR-Site.

Table 6-2. Direct dependencies between the process “Freezing” and the defined central area variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Central area geometry	Yes. Determines the total volume of water which can be frozen	The effects of freezing in the central area, ramp and shaft can be neglected based on the discussion in this section	No	The effects of freezing in the central area, ramp and shaft can be neglected based on the discussion in this section
Central area pore geometry	Yes.		Yes, redistribution of material	
Temperature	Yes. Obvious		No	
Water content	Yes, but freezing will always occur after full saturation		No	
Gas content	No. Not relevant		No	
Hydrovariables (pressure and flows)	Yes. The freezing point is affected by pressure		No flow in frozen water	
Stress state	No		Yes	
Central area materials – composition and content	Indirectly through pore geometry		No	
Central area porewater composition	Yes. The freezing point of water is affected by salinity		Yes. To a limited extent	
Structural and stray materials	No		No	

Boundary conditions

The only boundary condition for the process is the vertical temperature profile in the surrounding rock.

Model studies/experimental studies

No studies on materials to be used in the central area have been done.

Natural analogues/observations in nature

The described phenomena are well known from observations in nature.

Studies of changes in hydraulic conductivity due to freeze/thaw of coarse-grained materials, like moraine, show that hydraulic conductivity of a fine-grained glacial moraine, exposed to freezing and thawing, increased in the order of two orders of magnitude, e.g. /Johnston and Haug 1992/. It was concluded that the increase was mostly due to the amount of fines in the moraine. /White and Williams 1994/ has reported changes in hydraulic conductivity of 2-5 times for a silty moraine and /Viklander 1997/ increases in the order of 1-10 times for Swedish well-compacted moraines. The hydraulic conductivities reported are all measured in a direction parallel to the heat flow direction. Changes in hydraulic conductivity in a direction perpendicular to the heat flow are reported by /Chamberlain 1980/ and are in the same range as those parallel to the heat flow direction.

Time perspective

The process is relevant during the entire lifespan of the repository, although it only takes place during cycles of permafrost.

Handling in the safety assessment SR-Site

Due to the small amount of ice lens formation and the limited impact on the hydraulic conductivity on the material in central area, the process can be neglected.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

The references in this section are peer-reviewed publications available in the open literature.

Uncertainties

The uncertainty is related to the amount of clay and corresponding grain size distribution of the fill material. With higher clay content, the impact of freeze/thaw on the hydraulic conductivity will be greater.

6.2 Hydraulic processes

6.2.1 Water uptake and transport under unsaturated conditions

Overview/General description

Water transport in the crushed rock filled in the central area before saturation is mainly governed by the inflow rate and inflow distribution in the rock. Since the expected hydraulic conductivity of the crushed rock is rather high, and since there will be an open slot at the roof, the resistance to water inflow into the filling material will be very low.

In principle the hydraulic subprocesses are identical to those (A-E) described for the buffer (see Section 3.3.1) and will not be reproduced here. However, most processes connected with unsaturated water flow in the buffer and backfill are not relevant for the crushed rock. E.g. the suction in the crushed rock is insignificant and the temperature gradient is so low that there is no temperature driven vapour flow.

The only relevant processes for the crushed rock are the following:

- Transport of water in liquid phase, which is controlled and driven by
 - A1) a pressure gradient in the water,
 - A4) gravity (coupled to A1),
 - A5) a density gradient (coupled to A1).
 - Compression of
 - E2) air.
 - Transport in water of
 - F1) dissolved air.
- 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 porewater pressure u_w . Both of these can be described as functions of the void ratio e , the degree of saturation S_r and the temperature T .
- 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 can be an important process, especially in the ramp due to the high hydraulic conductivity.
- 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 the crushed rock, cf. process A1.
- 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. The crushed rock has such low suction that a pressurised air volume will remain if the air cannot seep out. A large part will disappear 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 room 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.

Dependencies between process and central area variables

Table 6-3 summarises how the process influences and is influenced by all central area variables and how these effects are treated in SR-Site.

Influence of pore geometry: The hydraulic behaviour depends very much on the grain size distribution of the crushed rock. If the percentage of fines ($<74 \mu\text{m}$) is low ($<10\%$), the hydraulic conductivity will be high ($K > 10^{-6} \text{ m/s}$) and there will be no relevant suction even at very low water content. If the rock is crushed and milled to a large portion of fines ($>30\%$), the hydraulic conductivity will be rather low ($K < 10^{-7} \text{ m/s}$) and there may be a relevant suction at low water content. However the density of the crushed rock and grain size sorting factor (well-graded or equigranular) also influence these properties significantly.

There are a number of factors influencing the hydraulic properties of crushed rock. The most important ones are

- Representative grain size (e.g. effective grain size $d_{10} = 10 \mu\text{m}$ meaning 10% weight of particles smaller than $10 \mu\text{m}$)
- Sorting coefficient (well-graded or equigranular)
- Dry density

Numerous suggestions of equations relating the hydraulic conductivity and the capillary rise to these and other parameters have been made. Figure 6-2 shows, as example, the relation between the hydraulic conductivity and the effective grain size d_{10} that can be used for rough calculations.

Table 6-3. Direct dependencies between the process “Water uptake and transport under unsaturated conditions” and the defined central area variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Central area geometry	Yes	Modelling	No	
Central area pore geometry	Yes. Via void ratio (density) and void geometry	Model parameters	No, but indirectly through hydro variables and erosion, if it takes place	See erosion, Section 6.2.4
Temperature	Yes. Through water viscosity and temperature gradient	Negligible	No, but indirectly through water content which affects thermal conductivity	Negligible
Water content	Yes. Via degree of saturation	Modelling	Yes	Modelling
Gas content	Yes. Via the gas pressure and degree of saturation	Modelling	Yes	Modelling
Hydrovariables (pressure and flows)	Yes. Basic.	Modelling	Yes	Modelling
Stress state	No		No	
Central area materials – composition and content	Yes. Hydraulic conductivity	Model parameters	No, but indirectly through hydro variables and erosion, if it takes place	See erosion
Central area porewater composition	Yes, small influence on viscosity and density	Negligible	Yes, settled by the inflowing water	No, the influence on the behaviour is negligible
Structural and stray materials	No		No	

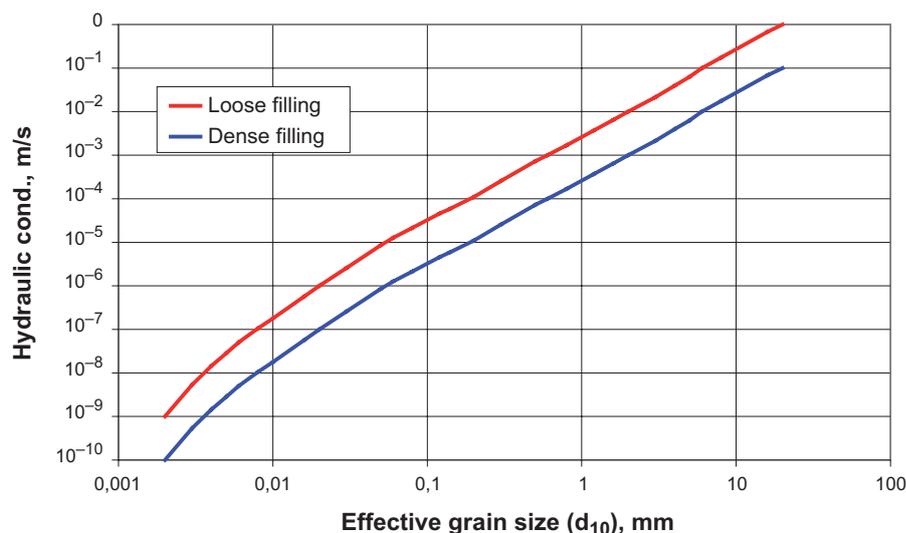


Figure 6-2. Relation between the hydraulic conductivity and the effective grain size d_{10} that can be used for rough calculations for rather even-grained soils /Fagerström and Wiesel 1972/.

The percentage of fines in the crushed rock is thus very important for the hydraulic conductivity. When TBM (Tunnel Boring Machine)-muck from TBM drilling is crushed, the percentage fines is rather high and (as shown below) the hydraulic conductivity can be very low. When rock from blasting is crushed, there will be no fines and the hydraulic conductivity is not expected to be lower than 10^{-5} m/s, unless grinding is performed.

If the percentage of fines is low and thus the hydraulic conductivity of the crushed rock is high and the suction negligible, the water saturation phase is expected to take place in a front like pattern, in the sense that the pores in the crushed rock are filled with water and will not fill the following pores until they are almost completely saturated. The influence of the degree of saturation on the flow rate is negligible.

If the percentage of fines is high and thus the hydraulic conductivity of the crushed rock is low, the suction may not be negligible if the initial water content is low. The water saturation rate may in that case be aided by the suction but, on the other hand, the hydraulic conductivity is for such a material lower and a function of the degree of saturation, which will delay the saturation.

A process that may strongly delay the saturation is when air has been trapped in the crushed rock. Since the water inflow is unevenly distributed, there may be many air pockets, especially at the roof in the central area, where there are no escape ways upwards.

Boundary conditions

Interaction with the rock: A key issue for the saturation process is the interaction between rock and central area. Water is conducted to the central area 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. The resistance to water inflow is low due to the high hydraulic conductivity of the crushed rock, so the inflow rate and saturation rate of the crushed rock is expected to be mainly governed by the rock hydrology and the natural inflow rate to the empty central area, ramp and shaft.

However, from highly water bearing fractures, the inflow rate may be so high that the crushed rock will prevent some inflow, which leads to an increased water pressure in the fracture. This could cause piping and erosion effects but should be possible to avoid by rock grouting.

Interaction with the tunnel plug: The crushed rock in the central area is in direct contact with the end plugs of the transport tunnels. Since the plugs are designed to seal off all water transport from the trunk and transport tunnels to the central area during the entire water filling and resaturation time, there will only be hydraulic interaction when full hydrostatic pressure has been reached.

However, since there is very little resistance against water filling from the rock into the central area filled with crushed rock, these parts may be water filled before the transport tunnels and full water pressure may act on the tunnel plugs before there is any counter pressure inside the plug. Since the plugs are not designed to withstand an elevated water pressure on the outside they may fail, in which case the tunnels will be filled by water from the central area.

Model studies/experimental studies

In Äspö HRL, there is a full scale test ongoing (Backfill and Plug Test) where the hydraulic properties of crushed rock as backfill material are investigated.

The *Backfill and Plug Test* /Gunnarsson et al. 2001/ includes tests of backfill materials and emplacement methods and a test of a full-scale plug. 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. Two different backfill materials are tested, namely a mixture of 30% bentonite and 70% crushed rock and 100% crushed rock. Rock debris from TBM drilling (TBM-muck) was used. Since TBM-drilling yields a large portion of fine material, due to the grinding process during drilling, the hydraulic conductivity of this material is very low.

The main objectives of the Backfill and Plug Test are

- to develop and test different materials and compaction techniques for backfilling 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 and 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 have been collected and reported. The plug has been 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. Hydraulic in situ tests of the section with crushed rock are still ongoing.

The hydraulic conductivity of the crushed rock has been investigated, but only after full water saturation /Johannesson et al. 1999/. The grain size distribution of the crushed rock material is shown in Figure 6-3 and the measured hydraulic conductivity as a function of the dry density is shown in Figure 6-4. The measured hydraulic conductivity is rather low due to the high content of fines ($d_{10} \sim 0.03$ mm), the sorting coefficient and the high dry density.

The retention curve that describes the suction of the material as a function of the water content has been measured. As shown in Figure 6-5, the suction is high at very low water content (<1%) but decreases fast with increasing water ratios and is negligible at the water ratio optimal (Proctor) for compaction (5-12%).

No model studies of the saturation phase of crushed rock have so far been done but hydraulic and hydrogeological modelling of the water filling will be done for SR-Site /Åkesson et al. 2010/.

Natural analogues/observations in nature

The grain size distribution of crushed rock reminds that of natural moraine soils. Many laboratory and field tests of such materials have been performed over the years and the results confirm the overall behaviour presented here. A general description of hydraulic behaviour of different coarse grained soils is given in /Fagerström and Wiesel 1972/.

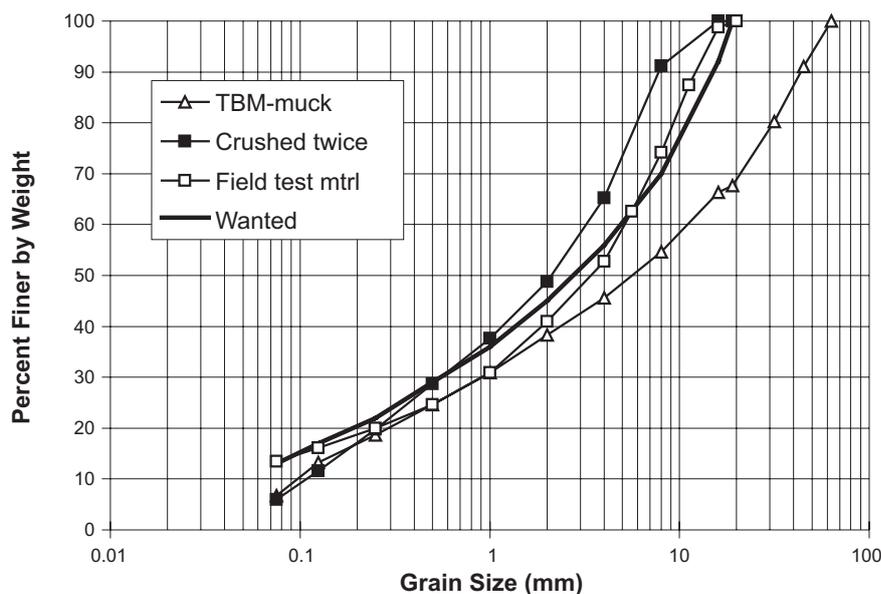


Figure 6-3. Grain size distribution of the natural uncrushed TBM muck, the ballast material used in the lab tests (Crushed twice) and the ballast material used in preparatory field tests /Johannesson et al. 1999/.

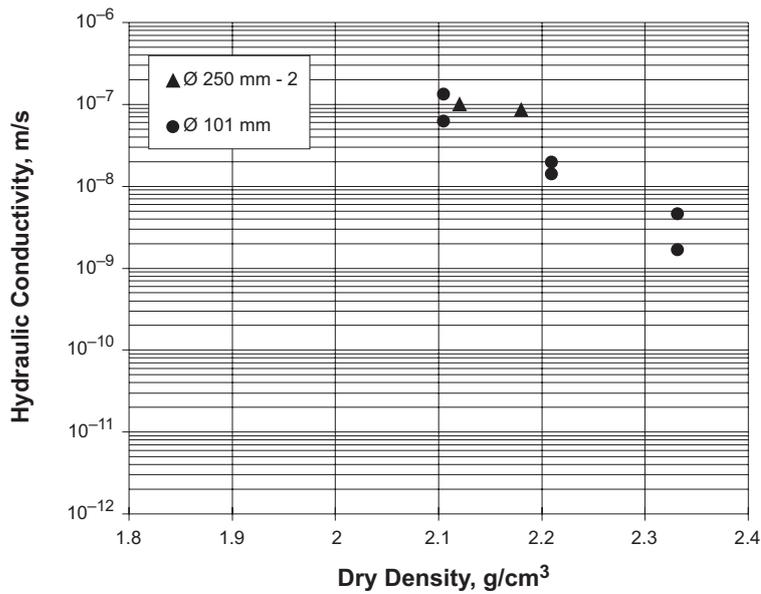


Figure 6-4. Measured hydraulic conductivity as a function of the dry density for crushed TBM muck (0/100) /Johannesson et al. 1999/.

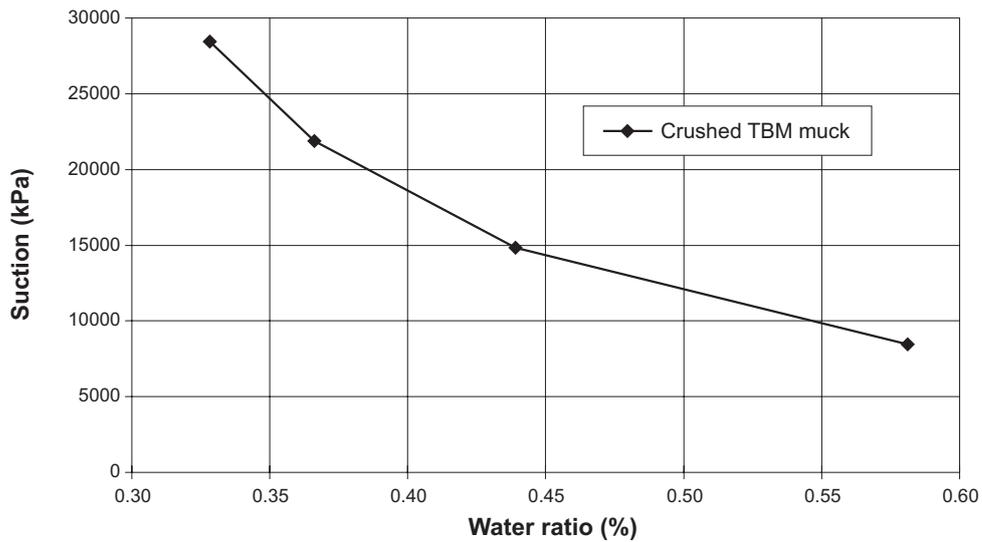


Figure 6-5. Measured total suction of crushed TBM muck as function of water content /Johannesson et al. 1999/.

Time perspective

Rough estimates show that the time to full water saturation of the central area can vary a great deal, depending, above all, on the hydraulic properties of the surrounding rock. In areas with rather high water inflow rates, saturation may be reached fast. If there are no fractures, all water has to go via the rock matrix, which may take considerable time in the granitic rock types occurring in Sweden. However, the time to reach full saturation will probably be shorter than that, since water may be transported along the rock surface from fractures located at other positions. In this case, full saturation is expected to be established in a few years, except where there are air pockets, which may remain for many years.

Handling in the safety assessment SR-Site

The inflow and successive water filling into these parts is modelled and the influence of different rock conditions is investigated with sensitivity analyses. This is done as a part of the THM modelling of the buffer, backfill and other system components /Åkesson et al. 2010a/.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

The inflow modelling will be reported in a general THM modelling report that will undergo a documented factual- and quality review /Åkesson et al. 2010a/.

The report describing the hydraulic conductivity of crushed rock by /Johannesson et al. 1999/ is not peer- or factual reviewed, but it is scientifically consistent with other references that are peer reviewed articles or papers.

Uncertainties

The basic hydraulic properties of the crushed rock in the central area are rather well known. The main uncertainties of these properties concern the risk and effect of piping.

Uncertainties in mechanistic understanding

The uncertainties are mainly related to the piping. The hydraulic model is well known.

Model simplification uncertainties in SR-Site

The model assumes that there is no piping.

Input data and data uncertainties in SR-Site

The model parameters need to be determined in detail when the material has been produced. The data used are discussed in the THM data report /Åkesson et al. 2010b/.

6.2.2 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. The general description of the water transport processes given in the previous section for unsaturated crushed rock is also valid under saturated conditions. In addition, the temperature gradient and salt content gradient may, after full pore pressure equilibrium is established, be an important factor for driving water flow due to the low natural pressure gradient.

After full water saturation and porewater equalisation, the main water transport in the central area will take place in the slot between the crushed rock and the roof. Such a slot will occur because of the difficulties in compacting crushed rock at the roof and because of the subsequent settlement of the material, unless the slot is filled with swelling material. The crushed rock in the shaft can, on the other hand, probably be compacted without leaving any open pathways, except for possible channels caused by piping.

Dependencies between process and central area variables

Table 6-4 summarises how the process influences and is influenced by all crushed rock variables and how these effects are treated in SR-Site.

The basic hydraulic properties of water saturated crushed rock are presented in the previous section.

Table 6-4. Direct dependencies between the process “Water transport under saturated conditions” and the defined central area variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Central area geometry	Yes	Modelling	No	
Central area pore geometry	Yes, void ratio (density) and void geometry	Model parameters	(Yes) If erosion takes place	See erosion Section 6.2.4
Temperature	Yes. Through water viscosity and temperature gradient	Neglected	Yes, by convection	Neglected
Water content	Yes. Hydraulic conductivity	Saturation assumed	No	-
Gas content	No	-	Yes	Saturation assumed
Hydrovariables (pressure and flows)	Yes. Basic variables.	Modelling	Yes	Modelling
Stress state	No	-	No	-
Central area materials – composition and content	Yes. Hydraulic conductivity	Model parameters	(Yes). If erosion takes place (secondary effect)	See erosion, Section 6.2.4
Central area porewater composition	Yes, via viscosity of water	Neglected	Yes	Neglected
Structural and stray materials	No	-	No	-

Influence of density, temperature and water salinity

The hydraulic conductivity is primarily dependent on the pore geometry, the composition of the crushed rock and the density. The ion concentration in the porewater and the temperature affect the hydraulic conductivity via the viscosity of the water but are of minor importance. They may, however, be important as pressure gradient generators.

Influence of other factors

After full water saturation and porewater equalisation, the open slot in the roof in the central area and the possible channels caused by piping are expected to dominate the behaviour unless the hydraulic conductivity of the crushed rock is very high. The very small pressure gradients will be further reduced since there is almost no flow resistance in these channels. This fact means that the pressure gradients caused by temperature differences and salt content differences may dominate the water transport.

Boundary conditions

Interaction with the rock: The water transport caused by the water pressure gradients in the rock fractures is dominated by the large fractures and fracture zones.

Interaction with the tunnel plug: The crushed rock in the central area is in direct contact with the end plugs of the transport tunnels. After long time when the plugs have been more or less disintegrated, there may be a direct hydraulic interaction also with the backfill material in the deposition tunnels, but the low hydraulic conductivity of the backfill strongly limits the hydraulic effect on the crushed rock.

Model studies/experimental studies

See Section 6.2.1.

Natural analogues/observations in nature

See Section 6.2.1.

Time perspective

The hydraulic gradient that exists after closure of the repository when water saturation and pore pressure equilibrium in the central area and surrounding rock have been reached is expected to be very low. Since the hydraulic behaviour will be dominated by open paths at the roof and along the rock wall from piping damages, it is expected that hydrostatic pressure will prevail in these parts. The hydraulic situation will be very sensitive to changes in hydrology on the ground surface.

Handling in the safety assessment SR-Site

The central area is an isolated part of the repository. However, the hydraulic conductivity can be high and there may be a need to include this feature in the hydrogeological model, at least as a sensitivity study.

Uncertainties

Uncertainties in mechanistic understanding

The hydraulic model for a high conductivity porous material is well known.

Model simplification uncertainty in SR-Site

The central area will be abstracted in to a section of the rock with very high hydraulic conductivity.

Input data and data uncertainty in SR-Site

All data used for this process will be pessimistic assumptions.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

The handling itself is a simplification to show sensitivity. The background reference for the overall understanding can be found in Section 6.2.1.

6.2.3 Gas transport/ dissolution

Overview/general description

Transport of gas in the central area can occur in two phases of the repository evolution:

1. Water saturation phase

The backfill consisting of crushed rock will be emplaced dry, 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 6.2.1

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 central area, ramp and shaft. The crushed rock backfill could act as a passageway for gas under certain conditions. However, it is not evident that gas from the canister will ever reach these areas. Gas release through the central area as well as the ramp and shaft is pessimistically neglected in SR-Site.

Dependencies between process and central area variables

The influence table for this process is in all important aspects identical to the table for the process “water transport under unsaturated conditions” (see Table 6-3)

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.

Model studies/experimental studies

The *Backfill and Plug Test* in the Äspö HRL /Gunnarsson et al. 2001/ includes a full scale test where the hydraulic properties of crushed rock as backfill material are investigated (see also Section 6.2.1). However, the information on trapped gas from that experiment is limited.

Natural analogues/observations in nature

Not applicable.

Time perspective

The delay of the water saturation of the crushed rock 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-Site

The influence of trapped air on the saturation time of the crushed rock backfill is investigated in SR-Site. The process involving trapped air is only relevant during the saturation phase (see Section 6.2.1).

The escape of corrosion gas from the canister through the crushed backfill is not considered in SR-Site.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

See 6.2.1

Uncertainties

The parameter values for the modelling 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.

6.2.4 Piping/erosion

Overview/General description

Water inflow into the central area will take place mainly through fractures and will contribute to the wetting of the crushed rock. However, if the inflow is localised to fractures that carry more water than the crushed rock can adsorb, there will be a build-up of water pressure in the fracture and therefore an increase in the hydraulic gradient through the crushed rock. If the total pressure from the water pressure in the fracture is higher than the resisting total pressure, the crushed rock will be deformed and an open channel or gap will be formed, where water can penetrate and continue to penetrate along the rock surface. This flow may also result in erosion of fine particles along the pipes. The processes are similar to the corresponding processes for the buffer described in Section 3.3.4.

The risk of **piping** depends on a number of factors the main ones being the following:

- The hydraulic conductivity of the crushed rock.
- The water inflow rate.
- The water pressure increase rate when water flow is stopped.
- The water inflow pattern (point wise or along a fracture).

The magnitude of erosion depends mainly on the grain size distribution and the percentage of fines in the crushed rock but of course also on the flow rate. Well graded crushed rock is less sensitive to erosion than equigranular. Piping and erosion will only take place during the water saturation phase. After porewater pressure equilibrium is established in the repository, the flow rate and water pressure gradients are too low. Erosion and how to avoid erosion is described e.g. in /Handboken BYGG /.

No self sealing of the crushed rock by swelling will take place.

Dependencies between process and central area variables

Table 6-5 summarises how the process influences and is influenced by all central area variables and how these effects are treated in SR-Site.

Boundary conditions

Piping and erosion in the crushed rock will take place at the interface between the rock and the back-filling. It will start at rock fractures and probably seek its way to the open slot at the roof if there is such a slot.

Table 6-5. Direct dependencies between the process “Piping/erosion” and the defined variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Central area geometry	Yes, limits the amount of eroded material.	Simplified calculations	No	-
Central area pore geometry	No, but indirectly through hydro variables.	Simplified calculations	Yes if erosion takes place	Simplified calculations
Temperature	No	-	No	-
Water content	Insignificantly	-	No	-
Gas content	No	-	No	-
Hydrovariables (pressure and flows)	Yes. Basic variables.	Simplified calculations	Yes	Simplified calculations
Stress state	Yes. The stress caused by the own weight of the crushed rock effects the piping	Simplified calculations	Insignificantly	-
Central area materials – composition and content	Yes both the risk of piping and the erosion	Hydraulic conductivity	(Yes). If erosion takes place	Simplified calculations
Central area pore-water composition	No	-	No	-
Structural and stray materials	No	-	No	-

Model studies/experimental studies

The processes are studied in conjunction with studies of the bentonite buffer and the bentonite back-fill materials. No model studies or experimental studies concerning crushed rock have been done so far. However, the problem of erosion is important for other engineering constructions (e.g. large dams for water power production) and a lot of information is available.

Natural analogues/observations in nature

Erosion has been observed and is a problem for many engineering constructions, especially large dams. One example is the failure of the Teton Dam in Idaho, USA, which was caused by piping and erosion of filling material under the dam /Seed and Duncan 1981/.

Time perspective

Piping and erosion in the crushed rock only takes place before complete saturation and porewater equilibration. The hydraulic gradient and resulting water flow rate is too low after equilibrium.

Handling in the safety assessment SR-Site

Piping and erosion could lead to a loss or redistribution of fine particles of the crushed rock in the central area, ramp and shaft. However, the consequence in the central area and ramp is considered not to affect the behaviour since the open slot at the roof will dominate. In the shaft, where no open slot is expected after emplacement and compaction, piping and erosion could significantly change the properties.

For the safety assessment, the central area will be considered to have direct hydraulic contact with its boundaries.

Uncertainties

Piping and subsequent erosion are complicated processes that probably are difficult to avoid in the crushed rock although a proper choice of grain size distribution could minimise the effect. However, since the backfill in the central area is assumed to have a high hydraulic conductivity under all circumstances in the safety assessment the uncertainties can be disregarded.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

No references are used.

6.3 Mechanical processes

6.3.1 Swelling/mass redistribution

This Section includes descriptions of all mechanical processes in the crushed rock in the central area except liquefaction. Thermal expansion, creep and a number of interactions with the end plug, the near-field rock and the top seal will be treated.

Overview/General description

The crushed rock has no swelling potential so mechanically it will only have a passive role. The interaction with the other parts will be governed by the stiffness and friction angle of the crushed rock.

The stresses in the crushed rock are rather low since they are only caused by the own weight of the material. In the central area the effective vertical stress (= total stress minus porewater pressure) varies from zero at the roof to 50-100 kPa in the floor, depending on the height of the rooms. The horizontal stress is about half the vertical one.

The **compressibility** (or stiffness) of the material can be expressed according to Equation 5-1.

$$M = \Delta\sigma/\Delta\varepsilon \quad (5-1)$$

where

M = compression modulus

σ = uniaxial stress with no lateral strain

ε = uniaxial strain with no lateral strain

The compression modulus can be determined with oedometer tests on the actual crushed rock. A test series have been performed on the crushed TBM-muck used in the Backfill and Plug Test at different densities (see Section 6.2.1).

If the compression modulus is evaluated between $\sigma=100$ kPa and $\sigma = 400$ kPa the compression modulus will be

$$M = 15\text{--}50 \text{ MPa}$$

These values are probably typical for crushed rock but depend on the grain size distribution, the shape of the grains and, especially, the dry density.

The **friction angle** is rather high. It depends on the same parameters as the compressibility. It was measured for the crushed TBM muck and was found to be $f=55^\circ$ for the dry density $2,200 \text{ kg/m}^3$ at the normal stress 1 MPa.

The influence of the degree of saturation can be neglected since the capillary pressure (suction) is very low.

Some settlement during water saturation and from long-term creep may also occur in the crushed rock although these effects are small due to the good compaction properties and high density that may be achieved after compaction.

Dependencies between process and central area variables

Table 6-6 summarises how the process influences and is influenced by all crushed rock variables and how these effects are treated in SR-Site.

Boundary conditions

The central area has three main mechanical boundaries, namely the plugs in the transport tunnels, the rock and the backfill at the ramp and shafts.

Interaction crushed rock / plug

There may be a mechanical effect on the crushed rock when the mechanical function of the concrete plug has ceased due to disintegration of the concrete. Then the swelling pressure from the backfill will be transferred to the crushed rock, yielding compression of a small part of the crushed rock and swelling of a small part of the backfill. The consequences can be estimated and are positive for the crushed rock, since the density will be further increased but also a loss in density of the tunnel backfill material will occur close to the plug.

Table 6-6. Direct dependencies between the process “Swelling/Mass redistribution” and the defined central area variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Central area geometry	No, influences indirectly the stresses		No	-
Central area pore geometry	Yes. Determines the density, which is important for the compressibility	Neglected, since mechanical effects are small and will have limited impacted	Yes affects the density	A hydraulic conductivity of the material is assumed in the hydrological model
Temperature	Insignificantly		No	-
Water content	No, via density (pore geometry)		Insignificantly	No
Gas content	Insignificantly		No	-
Hydrovariables (pressure and flows)	Insignificantly since they can only slightly delay the process		Insignificantly pore pressure will be equilibrated fast	A hydraulic conductivity of the material is assumed in the hydrological model
Stress state	Yes. Basic variable for mechanical processes	Neglected, since mechanical effects are small and will have limited impacted	Yes.	Neglected since it will have limited impact on the overall performance
Central area materials – composition and content	Yes. Determines stiffness and friction angle	Neglected, since mechanical effects are small and will have limited impacted	No	
Central area porewater composition	No		No	-
Structural and stray materials	Yes, corrosion of reinforcements may cause compression of the crushed rock both by volume expansion (negligible) and by loss of rock stability	Neglected, since mechanical effects are small and will have limited impacted	No	-

Interaction Crushed rock / Near field rock

The following mechanical interactions between the near-field rock and the backfill of crushed rock have been identified.

1. The lateral stress from the own weight of the crushed rock on the rock surface. It is small but may keep loosened rock pieces in place.
2. Stresses from detached rock pieces. Such pieces can affect the backfill of crushed rock, especially if they fall from the roof.
3. Convergence of the central rooms, ramp or shaft. This process compresses the backfilling and improves the properties.
4. Thermo-mechanical effects from heating and cooling the rock. The cooling phase will cause a small expansion of the open spaces. This will decrease the lateral stress from the backfill on the rock walls and will widen the gap at the roof, but the effect is small since the temperature changes are small in these parts.
5. Rock displacements from earth quakes or rock creep can locally affect the crushed rock.

Model studies/experimental studies

Backfill material of crushed rock has been used as one of two alternative backfill materials in the Backfill and Plug Test (see Section 6.2.1). The mechanical properties of this material have been tested in the field, 5-6 years after installation and water saturation with a 0.5 m diameter pressure cylinder that was installed in the floor of the tunnel. An oil pressure inside the cylinder was applied and stepwise increased up to 5 MPa during long time and the applied pressure and resulting deformation were measured. The results are shown in Figure 6-6. The test confirmed the very good mechanical properties of this material and showed that the achieved dry density after compaction was high. The total displacement at 5 MPa pressure was only about 2 cm.

Time perspective

Full saturation of the central area is expected to be achieved unevenly in a few years after closure of the repository and the hydraulic conductivity of the rock is the controlling factor. The degradation of the plugs, which may be fast if they collapse from high water pressure on the outside of the plug or take thousands of years due to dissolution of the concrete, creates a swelling pressure from the tunnel backfill on the inside of the plug. When porewater equilibrium has been reached, a small mechanical impact will come from the cooling phase.

In the long-time perspective, there is a (negligible) creep settlement of the crushed rock backfill and there may be local breakage of the near-field rock that is caused by high stresses, excavation damages and creep in the rock.

Natural analogues/observations in nature

No natural analogues concerning the mechanical behaviour of crushed rock backfill have so far been studied. The existence of relevant natural examples is probably very limited and would be difficult to evaluate. There are though some experiences from backfilling of mines.

Handling in the safety assessment SR-Site

Most of the mechanical effects related to mass redistribution are so small that they can be ignored in the safety assessment since the demands on the crushed rock backfill are low. The interaction between the crushed rock and the tunnel plugs is handled by a simplified model of both the effect of a sudden breakage of the plug and the swelling of the bentonite blocks in the plug after slow disintegration of the plug (see also Section 4.3.1).

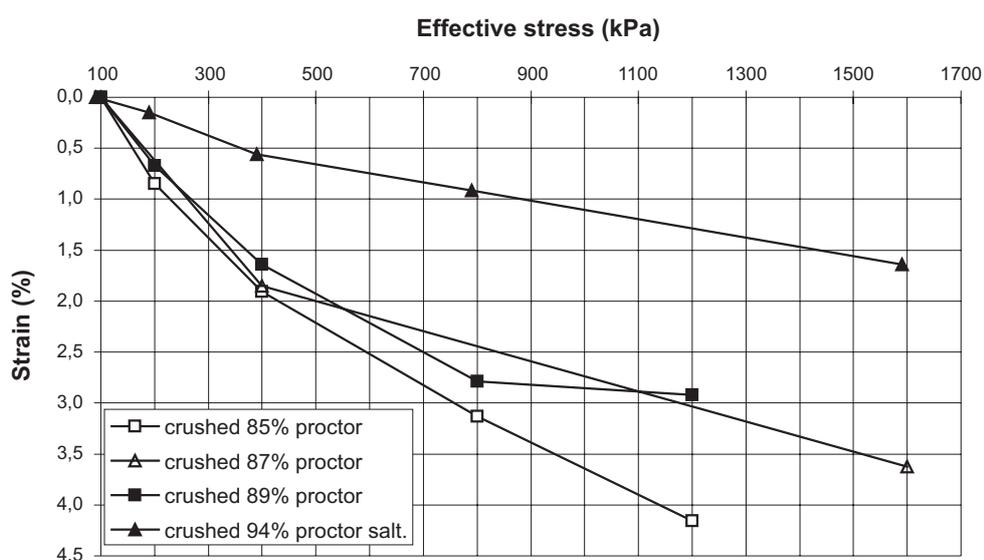


Figure 6-6. Results of the pressure cylinder test in the Backfill and Plug Test showing the displacement of the cylinder (red line) as a function of applied pressure. The stepped blue line is caused by delayed compression of the backfill due to consolidation effects (work in progress).

Modelling of the effect of tunnel plug disintegration (Section 5.3.1) is done for SR-Site and reported in the THM model report /Åkesson et al. 2010a/.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

Not applicable – the process is neglected in SR-Site.

6.3.2 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 porewater pressure is increased either due to a vibration that makes the sand particles float in the porewater (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 backfill of crushed rock that has been compacted, since the density is too high.

The consequences of liquefaction would anyway be negligible. The only conceivable effect is that a loose rock block in the roof may sink but the effect is local and does not affect the safety.

Handling in the safety assessment SR-Site

Since the process cannot occur and the consequences are negligible if it should occur, the process is neglected.

6.4 Chemical Processes

6.4.1 Advective transport of species

Overview/general description

In this context, advection refers to transport of any forms of additional matter, e.g. ions, molecules or colloids, with porewater flow. The transport direction is thereby principally from volumes of high water pressure to volumes of lower pressure. The process leads to redistribution of solutes in the porewater and thus affects the porewater composition. The advection is closely related to water flow in the central area, which is described in Section 6.2.2.

The backfill material in the central area consists of only crushed rock with a fuller distribution. The hydraulic conductivity is thereby relatively high ($>2 \cdot 10^8$ m/s). Advective flow will thereby be the dominant transport process in these repository components.

Table 6-7 summarises how the process influences and is influenced by all central area variables and how these effects are treated in SR-Site.

Boundary conditions

The external boundary condition for this process is the hydraulic and concentration gradient across the various repository components.

Table 6-7. Direct dependencies between the process “Advective transport of species” and the defined central area variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Central area geometry	Yes, major impact	Included in hydrogeological model	No	
Central area pore geometry	Yes, the density will influence the hydraulic conductivity	Included in hydrogeological model	No	
Temperature	Affects viscosity, Indirectly through temperature induced gradients and hydraulic conductivity. Freezing is of major importance	Neglected	No	
Water content	Yes, by definition	Saturated conditions assumed for transport calculations	No	
Gas content	Yes, dissolved gas is transported with flow. Indirectly through flow properties due to gas pressure, gas dissolution and precipitation.	Saturated conditions assumed for transport calculations	Yes, dissolved gas transported away	Saturated conditions assumed for transport calculations
Hydrovariables (pressure and flows)	Yes, by definition	Included in hydrogeological model	Yes, density effects may induce flow	Neglected
Stress state	No, or insignificant		No, insignificant	
Central area materials – composition and content	Yes, indirectly through sorption, precipitation and dissolution reactions	Included in hydrogeological model	No, indirectly through sorption, precipitation and dissolution reactions	
Central area pore-water composition	Yes, by definition	Only transport of water and radionuclides is considered	Yes, by definition	Only transport of water and radionuclides is considered
Structural and stray materials	No, indirectly through dissolution of concrete, reinforcement etc.		No, indirectly through deterioration of the materials	

Model studies/experimental studies

See Section 6.2.2

Natural analogues/observations in nature

See Section 6.2.2

Time perspective

Advective flow transport takes place on all timescales.

Handling in the safety assessment SR-Site

See Section 6.2.2

Handling of variables influencing this process:

See Section 6.2.2

Uncertainties

See Section 6.2.2

6.4.2 Diffusive transport of species

Overview/general description

A basic description of this process is given in Section 3.5.3. Since advection is expected to dominate in the crushed rock of the central area, see Section 6.4.1, diffusion is neglected.

Influence on variables of the central area: No influence on these variables is expected.

Boundary conditions

There are no particular boundary conditions to discuss for this process.

Model studies/experimental studies

Not relevant.

Time perspective

Not relevant.

Natural analogues/observations in nature

Through observations in nature (as well as in laboratory systems) it is well established that diffusion can be neglected in comparison to advective transport under the conditions (hydraulic conductivity and gradient) relevant for the central area; see e.g. /Grathwohl 1998/.

Handling in the safety assessment SR-Site

The process is neglected, since advective transport will dominate.

6.4.3 Sorption

Overview/general description

Radionuclides and major ions in percolating or porewater of the central area can be bound to the surfaces of the crushed rock material in several ways (see below). These processes are henceforth summarised under the term sorption and can affect the mobility of most radionuclides. The transport of major ions in the crushed rock is also influenced by these processes, which may influence the rate of weathering, see Section 6.4.3

In fresh crushed crystalline rock, the principal (primary or rock-forming) minerals offering surfaces relevant for sorption are micas. In comparison, the other major primary minerals in typical crystalline rock (quartz and feldspars) have a significantly smaller specific surface area and/or a lower concentration of relevant surface sites per unit mass. Upon exposure of the fresh surfaces to water, further surfaces of secondary minerals may be created as a result of weathering, such as clay minerals from feldspars or, under non-reducing conditions, Fe(III)-hydroxides from Fe in the crystal lattice of different primary minerals. Under reducing conditions, Fe(II/III) minerals (magnetite) or Fe(II) phases, such as siderite, may form. In weathered material, sorption will probably be dominated by the secondary minerals.

The principle type of surfaces offered by these minerals and the respective possible sorption reactions (surface complexation, ion exchange) are described in Section 3.5.5. Both mica as well as clay minerals are 2:1 layer silicates that consist of octahedral alumina sheets sandwiched between tetrahedral silica sheets, 1:1 clay minerals (kaolinite) may also occur. They differ in terms of layer charge and type of interlayer cation: 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 clay minerals. Clay minerals have a lower layer charge, with large hydrated cations (especially Na) occupying the interlayer space. Typically, this renders clay minerals expandable (exceptions are the 1:1 clays and 2:1 clays with a collapsed structure, such as illite), with a large interlayer surface area and higher CEC. Both minerals feature the same two types of distinctly different types of surfaces where two main types of sorption take place /e.g. Sposito 1984, Stumm and Morgan 1996/: i) planer siloxane or “layer” surface carrying a permanent charge and ii) variable charge, oxide-type edge surfaces with exposed AlOH and SiOH functional groups. The surfaces of Fe(III)-hydroxides and -oxides are similar to the edge surfaces of clays, but the exposed FeOH-groups typically show a higher affinity for many metal ions and reactive anions than clay edge surface groups /Dzombak and Morel 1990/. Further, hydrous forms of these minerals may (partly) re-crystallise over time, which can lead to the (irreversible) incorporation of adsorbed species. Because Fe is a redox-sensitive element, adsorbed species may also undergo redox reactions on these surfaces.

Dependencies between process and central area variables

Table 6-8 shows how the process influences and is influenced by all central area variables.

Influence on variables of central area, ramp and shaft: Exchange reactions of major cations directly influence the composition of the exposed surfaces of the crushed rock material as well as the porewater composition. It is also possible that changes in the porewater chemistry may induce changes in the surface composition of the crushed rock material through mineral dissolution and precipitation. However, bulk properties, including hydraulic conductivity, are not expected to be significantly altered by sorption and ion-exchange processes.

Influence of the composition of crushed rock and porewater: The two most important variables with regard to radionuclide sorption and exchange of major ions are the composition of porewater and of the crushed rock material. In case of the latter, sorption will be determined by the surface composition of the crushed rocks rather than by their bulk composition. I.e. sorption will be closely linked to weathering reactions. Based on the specific surface areas and sorption properties that are known for a range of relevant primary and secondary minerals, it appears to be likely that sorption will increase as weathering of the crushed rock material progresses. The porewater composition is the result of groundwater-rock 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. It can be expected that the mineralisation of percolating porewater will vary as a function of contact time with the rock surface (distance infiltrated) and as a function of the rock/water ratio or infiltration rate.

K_d is generally independent of the rock/water ratio per se. On the other hand, it can be expected that the sorption of radionuclides that mainly take part in ion-exchange reactions (Cs, Sr, Ra) will decrease with increasing mineralisation of the porewater. The sorption of other radionuclides (actinides, lanthanides, transition metals) is likely to increase with increasing pH (within the range of natural waters) and to decrease with an increase in the concentration of complexing ligands, such as dissolved carbonate.

Influence of temperature: As pointed out in Section 3.5.5, not enough sorption data as a function of temperature are available to clearly evaluate temperature effects. While an increase or decrease of the temperature (in comparison to room temperature) is potentially of importance for sorption, 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 porewater in the crushed rock material and the water in its adjacent components, i.e. mainly the boundary conditions of the process advection.

Table 6-8. Direct dependencies between the process “Sorption (including exchange of major ions)” and the defined central area variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Central area geometry	No	(total mass of crushed rock considered)	No	
Central area pore geometry	No (not on macroscopic scale)		No	
Temperature	Yes	Temperature effects neglected. Variations within expected temperature interval are covered by other uncertainties in sorption data.	No	
Water content	Yes (quantitative effect of solid/water ratio). Qualitatively possibly also indirectly through porewater composition	Sorption is expressed as K_d , whereby solid/water effect is cancelled out.	No	
Gas content	No, but in case of reactive gases: indirectly through porewater composition		No	
Hydrovariables (pressure and flows)	No, but possibly indirectly through porewater composition		No	
Stress state	No		No	
Central area materials – composition and content	Yes	Composition data used for estimate of sorption (see Geosphere process report, Sorption process /SKB 2010i/)	Yes, affects surface composition	Effect neglected (see Geosphere process report, Sorption process /SKB 2010i/) and section on alteration)
Central area porewater composition	Yes	Composition data used for estimate of sorption (see Geosphere process report, Sorption process /SKB 2010i/)	Yes	See Section 6.4.4, radionuclide concentration and release are calculated (see Geosphere process report, Sorption process /SKB 2010i/)
Structural and stray materials	Yes	Sorption on stray materials is conservatively excluded in SR-Site	No, but indirectly through porewater composition/mineral equilibria	

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 fresh and weathered crushed rock has been discussed above.

The effect of sorption on radionuclide transport has been discussed for clay systems in Section 3.5.5; this discussion is equally valid for the crushed rock material of the central area. On the other hand, effect of sorption on the properties of the crushed rock material can be neglected.

Time perspective

An ion exchange process in itself is normally very fast, so with respect to the distribution of major cations, the rates of other processes (dissolution/formation of minerals, transport of dissolved species) will control any apparent time dependency.

Surface complexation, which is the main sorption process for most radionuclides (see Section 3.5.5 and e.g. /NEA 2005, Dzombak and Morel 1990/), is a slower process than ion exchange; it may need up to several tens of days to reach equilibrium. The timescales that are of interest are thus dependent on the travel time of percolating water through the crushed rock material.

Natural analogues/observations in nature

Various well-researched examples exist regarding the interaction of radionuclides and major ions with unconsolidated, weathered rock /Davis et al. 2002, Davis and Curtis 2003/. These examples clearly show that sorption is dominated by and strongly dependent on the nature of the particular weathering products and on the composition of the contacting groundwater.

Handling in the safety assessment SR-Site

Sorption in the central area is pessimistically neglected in the transport modelling for the geosphere, see Geosphere process report, Sorption process /SKB 2010i/ for the justification.

Uncertainties

Uncertainties in terms of handling the process in SR-site are discussed in Geosphere process report, Sorption process /SKB 2010i/, data uncertainties in /Crawford et al. 2006/ and in the SR-Site Data report /SKB 2010l/. Uncertainties in mechanistic understanding are also discussed in Section 3.5.5.

6.4.4 Alteration of the central area backfill

Overview/general description

The geochemical evolution due to the interaction of groundwater with the crushed rock filling the central area is not expected to be very different than what it is expected from the groundwater interaction with the rock matrix or fracture-filling minerals Geosphere process report, processes: Reactions groundwater/rock matrix and Dissolution/ precipitation of fracture-filling minerals, /SKB 2010i/. The processes driving the geochemical evolution of these systems are mainly related to the dissolution – precipitation of minerals. Some of these reactions are relatively fast, as dissolution – precipitation of carbonate minerals and other fracture-filling minerals; whereas other reactions occur very slowly, limited kinetic dissolution rates (i.e. dissolution of most granite-forming silicates) and irreversible. All these reactions will control the composition of porewater that potentially can reach the near field of the repository system, especially considering that the central area may be a preferential pathway for groundwater (see Section 6.2.2).

Dependencies between process and central area variables

Table 6-9 shows how the process influences and is influenced by all central area variables.

Central area geometry: The central area geometry will determine the total mass of minerals able to react with porewater. In addition, these system parts will connect with water conducting fractures as well as with other parts of the repository, thus allowing that evolved porewater from the central area and the ramp and shaft can interact with these other system parts.

Central area pore geometry: The pore geometry in the central area will affect the geochemical behaviour of the system in several ways. First it will determine the solid/water ratio, affecting the reactivity of the system, i.e. more water is able to dissolve more minerals. The pore geometry will also affect the hydraulic conductivity, and therefore, changes in groundwater flow velocity will affect the dissolution – precipitation reactions, especially those reactions kinetically driven. Finally, the pore geometry affects the reactive surface of minerals, as rock fragments will have a larger reactive surface than surrounding rock matrix.

Table 6-9. Direct dependencies between the process “Alteration of the central area backfill” and the defined central area variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Central area geometry	Yes, important from mass-balance point of view, connects to water conducting fractures as well as to other repository parts	Included in modelling/evaluation (mass-balance)	No	
Central area pore geometry	Yes. Gives solid/liquid ratio Indirectly through hydraulic conductivity	Included in modelling	May be affected by dissolution precipitation	Neglected, since hydraulic conductivity always will remain high
Temperature	Yes, temperature effect on thermodynamic constants and kinetic rates.	Neglected since the temperature variations in the central area will be minor	No	
Water content	Yes, reactions only take place in the saturated domain.	Neglected, only saturated conditions are considered	No	
Gas content	No, but indirectly through water composition by affecting content of dissolved gases		Potentially, if a gas phase would form	Neglected, since the formation of a gas phase is of no concern
Hydrovariables (pressure and flows)	Yes, determines the turn-around rate of water	Included in modelling	No	
Stress state	No		No	
Central area materials – composition and content	Yes	Included in modelling	Yes	Included in modelling
Central area porewater composition	Yes	Included in modelling	Yes	Included in modelling
Structural and stray materials	Yes	Included in modelling	Yes	Neglected

The increase in reactive surface area of minerals and porosity will mainly affect the dissolution kinetic rates of both rock-forming minerals and fracture-filling minerals. As the present-day groundwater at repository depth has been interacting with all these minerals for a long period of time, increasing the surface area of such minerals will have a minor effect on the chemical composition of the groundwater. On the other hand, it is expected that initially, after filling the tunnels and shaft with crushed rock, all the void spaces will be filled with air, leading to an increase in the dissolution rate of those minerals able to oxidise (i.e. pyrite and iron-bearing silicates). Then, the increased mineral surface areas and the larger water-to-solid ratios will help to consume the oxygen faster, thus neutralising the possible effect of having oxidant waters at the repository depth.

Although the dissolution – precipitation of minerals can modify the pore geometry, the high initial total porosity is not expected to change significantly due to this process.

Temperature: Thermodynamic constants of chemical reactions are highly dependent of the temperature. However, temperatures in the central area are not expected to vary significantly, and therefore, minimal effects on the geochemical processes are foreseen.

Water content: Geochemical reactions are only expected to occur once this system part is saturated. Once the system is water saturated the effect of this variable will take place as described for the central area pore geometry variable.

Gas content: Gases can form or dissolve through chemical reactions, although their partial pressures are considered in the models, it is not expected that gases can form in these system parts. If gases from other system parts reach the central area, then they can dissolve in the relatively large volume of water, thus affecting the dissolution – precipitation of minerals.

Hydrovariables (pressure and flows): The high groundwater flow velocities expected in the central area and shaft will clearly affect the dissolution – precipitation reactions in the system, as porewater will be replaced relatively fast and dissolution can continue as equilibrium will be hardly achieved.

Stress state: This variable has no effect on the geochemical evolution process.

Central area materials – composition and content: This is one of the most relevant variables influencing this process. The type and amount of minerals is essential to determine how their dissolution – precipitation behaviour will affect the chemical evolution of the system, modifying both the porewater composition and the minerals present in the system (i.e. newly precipitated minerals and amount of existing minerals).

Central area porewater composition: The porewater composition will determine which of the minerals in the system will dissolve or precipitate, and thus the dissolution – precipitation of these minerals will modify the chemical composition of porewater. Moreover, changes in surface waters, as infiltration of ice-melting derived water, will very rapidly affect the chemical composition of the porewater, and hence the chemical evolution of the system.

Structural and stray materials: An additional aspect that can affect the geochemical behaviour of the crushed rock backfill is the presence of structural and stray materials. The time-length from the excavation of the repository until the use of excavated material as backfill will be relatively large. In this time frame it is expected that some biological activity take place in the depots where excavated material will be stored. Therefore, a certain amount of organic matter (i.e. dead animals and plants) will be present in the backfill material. Also the presence of other stray material (i.e. rejected metallic components) cannot be disregarded. The presence of such materials in the backfill can contribute to the geochemical evolution of the system, especially considering the likely activity of bacteria. Thus, the presence of organic matter can contribute to maintain the system under reducing conditions via the activity of sulphate-reducing bacteria and/or iron-reducing bacteria, or even, in the case of oxygen intrusion (i.e. ice-melting waters) due to the activity of aerobic bacteria see also Section 6.4.9. In this later case, it is worth noting that due to the larger hydraulic conductivity and porosity (compared to the surrounding rock) this will be a preferential path for surface waters, including ice-melting water during glaciation periods.

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 backfill water and the water in the adjacent geosphere and surface waters through the top seal above, i.e. the boundary conditions of the processes diffusion and advection.

Model studies/experimental studies

No specific studies of chemical processes in the crushed rock backfill of central area, ramp and shaft have been done. However, see also the description of the processes: Reactions groundwater/rock matrix and Dissolution/precipitation of fracture-filling minerals in the Geosphere process report /SKB 2010i/.

Natural analogues/observations in nature

No specific natural analogues have been investigated concerning the geochemical processes expected in excavated tunnels and backfilled with crushed rock. However, the processes will be equivalent to those occurring in organic matter-bearing aquifers, as gravel aquifers or backfilled abandoned mines where organic matter is present /Postma and Jakobsen 1996, Jakobsen and Postma 1999, Banwart 1999, Hartog et al. 2004, Massmann et al. 2004, Park et al. 2006, Jakobsen and Cold 2007/. In these systems, reducing conditions are maintained through different types of bacterial mediated organic matter degradation reactions. The specific type of organic matter degradation depends on the type and amount of organic matter as well as on the dominant electron acceptor in groundwater.

Time perspective

The processes considered are of relevant importance at different timescales. In early stages after repository closure (once the crushed rock backfill is emplaced) the processes involving oxygen consumption from trapped air will be the most relevant. Once the reducing conditions are restored, the water – rock interaction processes will continue for the whole repository life-span. A special case is related to the intrusion of ice-melting derived water and penetration of oxygen to repository depths. In this case, the processes involving oxygen consumption will be constrained to the glaciation – deglaciation timescales.

Handling in the safety assessment SR-Site

The geochemical evolution in the crushed rock backfill of the central area is evaluated through a reactive transport equilibrium or mass-balance model, where the processes in this system component are implemented together with transport processes (advection). Two different time periods have to be evaluated, one for the initial times (during the water saturation after backfilling until a chemical stationary state is reached) and the other considering the response of the system to the intrusion of ice-melting water (glaciation – deglaciation timescales) from the top and assuming the system is fully saturated.

Initially, the system is assumed to be unsaturated and the pore space filled with air and thereafter the system gradually saturates with present-day groundwater from the tunnel walls and surface water from the surface. The evolution of the system has to consider the consumption of dissolved gases in equilibrium with atmosphere conditions (i.e. $p\text{CO}_2 = 10^{-3.5}$ bar and $p\text{O}_2 = 10^{-0.7}$ bar) and how these dissolved gases affect the dissolution – precipitation of rock-forming and fracture-filling minerals present in the system. Moreover, the effect of organic matter degradation has to be considered, first through oxidation reactions involving aerobic bacteria and, once oxygen has been consumed, through reactions involving sulphate-reduction or iron-reduction bacteria. The evolution of the system has to be assessed in order to evaluate the oxygen consumption and to determine the stationary redox state of the system.

The second part of the system evaluation has to consider a glaciation – deglaciation time period, where oxygen-rich ice-melting water can intrude the system from the surface. In this case, full saturation can be assumed (i.e. the output conditions from the previous case) and the water-rock reactions consuming oxygen, including organic matter degradation, implemented in the model. This will allow assessing the penetration depth of oxygen and the potential impact on the repository, as well as the redox buffering capacity of the system.

Handling boundary conditions:

Two main boundary conditions have to be considered. One is the transport conditions from tunnel walls into the backfilled system and the other is the composition and flow conditions of surface water entering into the system from the surface.

Transport conditions have to be handled according to the process advection. Initial chemical compositions of both groundwater and surface water (including ice-melting derived water) will be based on the hydrogeological modelling, see Section 6.2.2.

Handling influences between variables and process:

Groundwater flow and composition are defined as part of the boundary condition as stated above. The volume and porosity of the central area is considered and fracture and matrix minerals are fully included in the modelled system, as well as stray materials. The saturation phase is neglected in the geochemical model, since it is short in duration and will have limited impact.

Handling coupling to other processes:

The model here considered only includes the coupling with transport processes as well as with the microbial activity.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

All the references cited are peer reviewed papers except the Geosphere Process Report /SKB 2010i/, which is a SKB Quality Assured report.

Uncertainties

Uncertainties in mechanistic understanding

Some critical uncertainties remain concerning the mechanistic understanding of the processes that control the redox state of the system. These are mainly related to the degradation of organic matter. Although a generic organic matter and mass-balance can be used (CH_2O), the lack of knowledge on the mechanistic degradation of the specific organic matter could introduce a large uncertainty to the system.

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 the considered conditions is poor. This is mainly related to the dissolution of rock-forming silicates and their transformation into clay minerals. Although these reactions occur at a very slow rate, their effect on the overall geochemical evolution is not yet clear.

Model simplification uncertainty in SR-Site

There are several rock-forming minerals, such as silicates other than silica, which tend to dissolve at a very slow kinetic rate and irreversibly. Other silicates (usually clay minerals) precipitate at similarly slow rates. However, the dissolution-precipitation processes involving these two groups of minerals could affect the pH evolution of the system as well as the chemical composition of the groundwater, thus affecting the chemical long-term evolution of the system.

Modelling of chemical reactions driven by microbial activity generally makes use of kinetic rates for organic matter degradation. The computed rates are generally fast as compared with the timescale of reactions with rock-forming minerals. The results of the modelling are strongly coupled to the microbial processes considered and to the values of the parameters used. The introduced simplifications, such as considering a generic organic matter (i.e. CH_2O), could result in differences with respect to actual rates of oxygen consumption.

Input data and data uncertainty in SR-Site

Another source of uncertainty relates to the quantitative estimation of sensitive parameters associated with microbial kinetics, such as growth rate and half saturation constants in the kinetic expressions. Such parameters are both microbe dependent and environment dependent. Usually, parameter values are obtained in laboratory conditions by means of physiological (i.e. growth) in vitro experiments which cannot be fully representative of repository conditions. Results of current in situ microbe investigations, as well as model calibration based on field experimental data could be helpful for the up-scaling of key microbial parameters. Nevertheless, model calculations involving microbial processes, even if they are calibrated against experimental field data, are necessarily of qualitative value.

6.4.5 Alteration of concrete components

Overview/general description

In the central area, cement-bearing materials can be present as construction concrete and grout can remain in the system after backfilling this system part. The alteration of such materials can affect the system in two different ways: 1) as a consequence of its degradation the porosity can increase, thus creating favourable pathways for groundwater to enter into the system, and 2) the increase of alkalinity due to the interaction of groundwater with these materials can enhance the dissolution rate of smectite (Section 4.4.7 in Backfill chapter and Section 3.5.9 in Buffer chapter), weakening the effectiveness of the bentonite backfill in the deposition tunnels as a hydraulic barrier.

The processes associated to the alteration of concrete components are equivalent to those considered for concrete in the tunnel plug (Section 5.4.4).

Handling in the safety assessment SR-Site

The degradation of the concrete in the central area is assumed to be equivalent with the degradation of the concrete part of the tunnel plug (Section 5.4.4). No separate modeling will be done.

6.4.6 Aqueous speciation and reactions

Overview/general description

This process is in general the same as the corresponding process in the buffer (Section 3.5.7.)

Handling in the safety assessment SR-Site

The process is included in a separate modelling task of the central area geochemical evolution. This is further described in Section 6.4.4.

6.4.7 Osmosis

Overview/general description

The general process is described for the buffer system in Section 3.5.8. In the crushed rock the effect will be insignificant since the material itself will not have a semipermeable behaviour.

Handling in the safety assessment SR-Site

The process is neglected since osmotic effects will be insignificant in the crushed rock material.

6.4.8 Corrosion of steel components

Overview/general description

Steel in the reinforcements in the central area will not be stable under repository conditions. Corrosion of steel is described in the Canister Process Report /SKB 2010k/. The main resulting products will be some type of iron-oxide and hydrogen gas. Neither of the corrosion products is assumed to have any negative impact on the repository performance.

Handling in the safety assessment SR-Site

The total amount of steel is included in all mass-balance calculations of effects of microbial activity, see Section 6.4.9. The corrosion rate of steel reinforcements will pessimistically be neglected.

6.4.9 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 /Madigan et al. 2008/. From a microbiological perspective, the central area environment will constitute an environment with mixed characters from two other well defined environments of the repository concept; the geosphere and the buffer. The central area environment will, however, have some characteristics that significantly distinguish them from the two other mentioned environments. One is the presence of organic material in structural and stray material. Another is the gas/water interface that will develop during the saturation process and hydrogen formation from anaerobic corrosion of rock bolts and nets. The effects of microbial processes on the chemical stability of the geosphere have been thoroughly discussed /SKB 2010i-microbial processes/. Similar effects can be obtained in the backfill, but the differences in the variables “structural and stray materials and the gas content” compared to the geosphere may introduce some additional effects that must be considered.

Plasticisers that will be added to grout and shotcrete commonly contain organic polymers of varying compositions, e.g. polycarboxylate polymers. The amounts to be used will be significant, in the range of 100 tonnes or more as exemplified in /SKB 2010g/. Plasticisers introduce a significant uncertainty, because their composition and solubility, and thereby their availability to microbes, are not well known. In cases where a grouting activity fails and the grout do not solidify properly; large amount of organic carbon will be available for microbial growth. Such growth can occur in the grouted aquifers and in the central area, ramp and shaft on places where groundwater from grouted sites seep through the tunnel walls. There are two main influences from the structural material variable on microbial processes.

1. Microbial sulphate reduction during microbial growth on plasticisers will result in sulphide. The sulphide may accumulate as iron sulphide in slime formations on the shotcrete and on rock tunnel walls. During the open phase, oxygen will oxidize the sulphide and sulphuric acid can form. Local acid attacks on the shotcrete will occur. This effect will diminish after backfilling, when oxygen is consumed, but it may introduce a safety concern during the open phase.
2. Excess amounts of organic material in aquifers will trigger growth of opportunistic microorganisms that will increase in numbers. Several groundwater microorganisms produce complexing agents that very efficiently mobilize trace elements, including many radionuclides /Kalinowski et al. 2004, 2006, Johnsson et al. 2006, Essén et al. 2007, Moll et al. 2008/. Given the large amount of added organic carbon where grouting have been performed, it is possible that the microbial production of complexing agents will be significant which may notably reduce the retardation effects accounted for by the rock and the rock matrix.

Dependencies between the process and the tunnel plug variables

Table 6-10 shows how the process influences and is influenced by all central area variables.

Boundary conditions

The access to organic material, e.g. stray materials and construction material such as organic additions to the grout and shotcrete, hydrogen from anaerobic corrosion of iron, organic material from other material that cannot be stripped or cleaned out and methane and electron acceptors from the geosphere will set the limits for the microbial processes in the central area, ramp and shaft. Given the large amount of plasticizer that will be added, access to organic carbon can be assumed for a very long time.

Model studies/experimental studies

None.

Natural analogues/observations in nature

No directly relevant natural analogues or observations are known.

Table 6-10 Direct dependencies between the process “Microbial processes” and the defined Central area variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Central area geometry	No		No	
Central area pore geometry	No		Growth of microbes generate biomass that may clog pores	This effect is not considered in SR-Site
Temperature	Yes, microbial activity increases with temperature	This effect is not considered in SR-Site	No	
Water content	Yes, availability of water	Saturated conditions assumed	No	
Gas content	Indirectly through water content		No	
Hydrovariables (pressure and flows)	Yes, water is needed for growth of microbes and growth on hydrogen and methane is possible. Pressure is not important	This effect is not considered in SR-Site	Yes, microbes may form methane and hydrogen	This effect is not considered in SR-Site
Stress state	No		No	
Central area materials – composition and content	Yes, the content of organic carbon and microbes in different backfills varies	This effect is not considered in SR-Site	No	
Central area porewater composition	Yes, microbes are sensitive to the geochemical situation, and may utilise porewater components for growth	This effect is not considered in SR-Site	Yes, microbial activity may change the composition, e.g. by consumption of methane, sulphate and organic carbon and production of sulphide and carbon dioxide.	This effect is not considered in SR-Site
Structural and stray materials	Yes, organic components in grout and hydrogen from anaerobic iron corrosion will constitute sources for microbial growth.	Production of microbial biofilms, acid and complexing agents from organic carbon in grout is considered in SR-Site	Yes, microbes may oxidise organic components in this material.	This effect is not considered in SR-Site

Time perspective

Microbial processes will start when water becomes available. The process rates will be largest in areas where organic carbon and hydrogen are available. Elevated microbial process rates, compared to the geosphere, will continue until all sources for growth have been consumed.

Handling in the safety assessment SR-Site

Microbial reactions will be considered in the description of the geochemical evolution in the central area. This is done with mass-balance considerations.

Handling of uncertainties in SR-Site

Microbial degradation of organic carbon and consumption of hydrogen from metal corrosion will be considered in the modeling of the geochemical evolution repository. This will be done through a combination of thermodynamic, kinetic and mass balance models/assumption.

Uncertainties in mechanistic understanding

The amount of hydrogen from anaerobic iron corrosion and the amount of organic material from grouting that becomes available for microbial growth and activity is unknown.

Model simplification uncertainty

Not relevant since no quantitative model for microbial processes in the backfill is used.

Input data and data uncertainty

Not relevant since no quantitative model for microbial processes in the backfill is used.

6.4.10 Colloid release

Overview/general description

Fractures intersecting the central area mean that rigid volumes restrictions are not present everywhere, and that small-sized material may enter the fractures. Separation of individual particles from the introduced material may then take place (dispersion).

The behaviour of the particles will be dominated by thermal motion if the particles are small enough i.e. they have colloidal properties. The individual colloidal particles may then be transported away from the tunnels into fractures by diffusion or by groundwater flow in the fractures.

The magnitude of the process is governed by the size distribution of the crushed rock. The material can be chosen in such a way that colloid formation may be neglected.

Handling in the safety assessment SR-Site

The process is neglected due to the very small possible effect, also for the unlikely case that all particles of colloidal size are transported away. No credit is taken for the fine particles under any circumstances and the hydraulic conductivity is assumed to be high under all circumstances.

6.4.11 Radiation induced transformation

Overview/general description

The central area is too far away from the canisters to be affected by the g-radiation. The effect of a-radiation from radionuclides from damaged canisters can also be neglected, since the levels will be extremely small (see Section 3.5.12).

Handling in the safety assessment SR-Site

The process is neglected.

6.5 Radionuclide transport processes

6.5.1 Speciation of radionuclides

Overview/general description

See corresponding process description for the buffer, Section 3.6.1

Handling in the safety assessment SR-Site

This process is indirectly handled through the selection of parameters for radionuclide transport in the rock. In general, the handling of the process is the same as for the corresponding process in the geosphere, see process transport of radionuclides in the water phase in the Geosphere Process Report /SKB 2010i/.

6.5.2 Transport of radionuclides in the water phase

Overview/general description

The central area is represented as a volume with high hydraulic conductivity and high porosity in the geosphere transport model.

Handling in the safety assessment SR-Site

Delay of radionuclides in the central area is pessimistically neglected. See process transport of radionuclides in the water phase in the Geosphere Process Report /SKB 2010i/.

7 Processes in the top seal

7.1 Thermal processes

7.1.1 Heat transport

Overview/general description

At the bottom boundary of the top seal, the rock peak temperature occurs about 1,000 years after deposition, and will be between 5 and 7°C above the initial temperature at 100 m below ground surface, and correspondingly smaller at shallower depths /Hökmark et al. 2009/. The volume of the top seal is small enough for its thermal evolution to be completely controlled by the slow and modest change in the temperature of the surrounding rock mass, regardless of the heat transport properties of the top seal materials. The modest temperature variations cannot influence the variables in any way that impacts on the performance of the top seal. Therefore, the process heat transport in the top seal is not addressed further.

Handling in the safety assessment SR-Site

The process is neglected.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

The reference /Hökmark et al. 2009/ will undergo a documented factual and quality review.

7.1.2 Freezing

Overview/general description

The top seal of the shafts from ground surface down to approx. 100 m depth will be filled with big boulders. The size of the boulders will be in the range of metres. During freezing periods, the water between the boulders will be frozen and the system will have temperatures well below 0°C. When water undergoes phase change to ice, energy is released (333 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. 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, Nersesova and Tsytoich 1965, 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.

In a very coarse-grained material, like boulders, the amount of unfrozen water is negligible due to the very small specific surface in the system and corresponding big voids between particles. In relation to the salt content of the water, the porewater turns into ice at temperatures close to 0°C. As the unfrozen water content is negligible, this means that all water freezes to ice at the same temperature, i.e. close to 0°C.

During freezing, water expands. In a system with high hydraulic conductivity, the expansion during freezing will expel water out of the pore system at the same rate as water expands during the ice forming process. Neither volume increase nor stress increase of the system will take place as long as water can be expelled in an open system. No ice lensing with accompanying frost heave will take place, as the unfrozen water content will be negligible and thus no suction will be developed.

Frost penetration rates in ground, relevant for frost penetration due to low temperatures at the ground surface, are at most in the range 2-3 m/year.

A freezing ground can be regarded as an open system if the hydraulic conductivity is greater than 10^{-5} m/s (conservative value) for normal freezing rates. A very coarse-grained material like boulders will have a hydraulic conductivity of about 10^{-1} m/s and therefore no frost phenomena will be present.

Particles of rock materials will be affected by freezing if fractures are present in the particles before freezing and thawing and the particles stay in a water-saturated environment. Water having penetrated into open fractures and voids in the particles will expand, and if the fractures are small, or if freezing takes place in a direction that closes the entry of the fractures, an open system will not be present in the particle itself. High pressures can build up thus causing cracking of the particle. The phenomenon is known from nature as frost cracking. The process goes on until solid parts of rocks, without fractures, remain. Particles without cracks will not be affected by freezing. This is also well known from nature.

The boulders used as top seal will thus be affected as they to some extent will have cracks. The material will be successively finer and the end result of the particle size will be dependent on the amount of cracks in the material used. Boulders of granite or similar hard rock will not end up in a smaller material than gravel and stones. If the boulders initially are free of fractures, freezing will not affect the material.

Dependencies between process and top seal variables

Table 7-1 shows how the freezing process influences and is influenced by all top seal variables.

Table 7-1. Direct dependencies between the process “Freezing” and the defined top seal variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Top seal geometry	Determines the total volume of water which can be frozen	The effects of freezing in the top seal can be neglected based on the discussion in this section	No	The effects of freezing in the top seal can be neglected based on the discussion in this section
Top seal pore geometry	Yes		Yes, redistribution of material	
Temperature	Obvious		No	
Water content	Yes, but freezing will always occur after full saturation		No	
Gas content	Not relevant		No	
Hydrovariables (pressure and flows)	The freezing point is affected by pressure		No flow in frozen water	
Stress state	No		Yes	
Top seal materials – composition and content	Yes, the clay content of the backfill affects the freezing		No	
Top seal porewater composition	The freezing point of water is affected by salinity		To a limited extent	
Structural and stray materials	No		No	

Boundary conditions

When the top seal is frozen, no stress increase or expansion of the system will be present as long as the frost penetration in the material is less than 100 m per year. In natural freezing, frost penetration is less than in the order of 2-3 m/year.

The particles will be affected by freezing and particle size of the boulders, after hundreds of freezing cycles, will be in the range of stones.

Model studies/experimental studies

No specific studies on freezing of top seal materials have been done.

Natural analogues/observations in nature

The described phenomena are well known from observations in nature.

Time perspective

The process takes place during cycles of permafrost.

Handling in the safety assessment SR-Site

Due to the high hydraulic conductivity of the top seal, no stress increase or expansion will take place. The process can therefore be neglected.

Particles will be affected and broken into smaller pieces. The final condition will be particles of stone size. This can have an effect on the accessibility to the repository.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

The references in this section are peer-reviewed articles from the open literature or engineering handbooks.

Handling of uncertainties in SR-Site

The uncertainty is related to the size of the boulders after a large number of freezing and thawing cycles. The end product can be bigger than stones but not very much smaller. How the size of the particles in the top seal affect the accessibility to the repository has to be evaluated.

7.2 Hydraulic processes

7.2.1 Water uptake and transport under unsaturated conditions

Overview/General description

Water transport in the crushed rock filled in the top before saturation is mainly governed by the inflow rate and inflow distribution in the rock. Since the expected hydraulic conductivity of the crushed rock is very high and since there may be an open slot at the roof in the ramp, since the backfill material has no swelling properties, the resistance to water inflow into the filling material will be very low.

In principle the hydraulic subprocesses are identical to those (A-E) described for the buffer and will not be reproduced here. However, most processes connected with unsaturated water flow in the buffer and backfill are not relevant for the crushed rock. E.g. the suction in the crushed rock is insignificant and the temperature gradient is so low that there is no temperature driven vapour flow.

The only relevant processes for the crushed rock are the following:

- Transport of water in liquid phase, which is controlled and driven by
 - A1) a pressure gradient in the water,
 - A4) gravity (coupled to A1),
 - A5) a density gradient (coupled to A1).
 - Compression of
 - E2) air.
 - Transport in water of
 - F1) dissolved air.
- 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 porewater pressure u_w . Both of these can be described as functions of the void ratio e , the degree of saturation S_r and the temperature T .
- 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.
- 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 the crushed rock, cf. process A1.
- 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. The crushed rock has such low suction that a pressurised air volume will remain if the air cannot seep out. A large part will disappear 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.

Dependencies between process and top seal variables

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

The hydraulic behaviour depends very much on the grain size distribution and the density of the crushed rock. Since the exact values of hydraulic conductivity are not determined and since there are no demands on the hydraulic conductivity it is assumed that it is so high that the top seal filling material is filled with water at the same rate as it enters from the fractures in the rock and flows downwards until the water comes into contact with the underlying less permeable backfill. Part of the water will then flow into this backfill and part will stay and fill up the top seal. The blasted and crushed rock used for the top seal is expected to have a hydraulic conductivity of 10^{-1} m/s or higher.

A process that could delay the saturation is when air has been trapped in the top seal. However, the trapped air will disappear upwards since there is virtually no capillary forces that entrap the air and since there is a free way upwards towards the atmosphere.

Boundary conditions

Interaction with the rock: The high hydraulic conductivity of the top seal material makes the inflowing water flowing downwards and filling up the ramp or shaft.

Interaction with the atmosphere: The upper part of the top seal will connect and adapt to the groundwater system in the biosphere.

Interaction with the backfill underlying the top seal: There will be a hydraulic contact between these parts and some of the inflowing water may be lost downwards in the beginning.

Table 7-2. Direct dependencies between the process “Water uptake and transport under unsaturated conditions” and the defined top seal variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Top seal geometry	Yes	Considered in inflow estimates.	No	
Top seal pore geometry	Yes. Via void ratio (density) and void geometry	Considered in inflow estimates.	No	
Temperature	Yes.	Neglected. Insignificant	Yes.	Neglected. Insignificant
Water content	Yes. Via degree of saturation	Neglected. Insignificant.	Yes	No. Insignificant.
Gas content	Yes. Via the gas pressure and degree of saturation	Neglected. Insignificant.	Yes	No. Insignificant.
Hydro variables (pressure and flows)	Yes. Basic.	Considered in inflow estimates.	Yes	No. Insignificant.
Stress state	No		No	
Top seal materials – composition and content	No, but indirectly through hydro variables (Hydraulic conductivity)	See row hydro variables	No	
Top seal porewater composition	No		No	
Structural and stray materials	No		No	

Model studies/experimental studies

No studies of these kinds have been performed, but there is a solid knowledge of the hydraulic behaviour of fillings with crushed or blasted rock.

No model studies of the saturation phase of crushed rock have so far been done but the rate of water filling and the interaction with the underlying crushed rock should be calculated.

Natural analogues/observations in nature

Not required since the process is well known.

Time perspective

The time it takes to fill up the top seal with water depends on the inflow rate from the rock and the loss of water to the underlying backfill. However, it is probably a matter of years and not decades.

Handling in the safety assessment SR-Can

This process is only handled by a rough estimate of the time it may take to fill the top seal with water.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

Water flow in sand and crushed rock fillings are well known and demonstrated in numerous examples. See e.g. /Handboken Bygg/ and /Cederwall and Larsen 1976/ as well as /Pusch 2008/.

Uncertainties

The hydraulic properties of the blasted and crushed rock in the top seal will be known well enough when the laboratory tests on the actual material can be done.

Uncertainties in mechanistic understanding

None.

Model simplification uncertainties in SR-Can

Not relevant.

Input data and data uncertainties in SR-Can

Not relevant.

7.2.2 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. The general description of the water transport processes given in the previous section for unsaturated crushed rock is also valid under saturated conditions. In addition, the temperature gradient and salt content gradient may after full pore pressure equilibrium be an important factor for driving water flow due to the low natural pressure gradient.

Dependencies between process and top seal variables

Table 7-3 summarises how the process influences and is influenced by all top seal variables and how these effects are treated in SR-Site.

Influence of density, temperature and water salinity: The hydraulic conductivity is primarily dependent on the pore geometry, the composition of the crushed rock and the density. The ion concentration in the porewater and the temperature affect the hydraulic conductivity via the viscosity of the water, but are probably of minor importance. They may however be important as pressure gradient generators.

Influence of other factors

After full water saturation and porewater equalisation, the natural pressure gradient is small. This means that the pressure gradients caused by temperature differences and salt content differences may dominate the water transport.

Boundary conditions

Interaction with the rock: The water transport caused by the water pressure gradients in the rock fractures is dominated by the large fractures and fracture zones.

Interaction with the atmosphere: The upper part of the top seal will connect and adapt to the groundwater system in the biosphere.

Interaction with the backfill underlying the top seal: There will be a hydraulic contact between these parts.

Model studies/experimental studies

No studies of these kinds have been performed but there is a solid knowledge of the hydraulic behaviour of fillings with crushed or blasted rock.

Table 7-3. Direct dependencies between the process “Water transport under saturated conditions” and the defined top seal variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Top seal geometry	Yes	Included in the hydrogeological large-scale model	No	
Top seal pore geometry	Yes. Via void ratio (density) and void geometry	Model parameters	No	
Temperature	Yes. Through water viscosity and temperature gradient	Insignificant	Yes, by convection	Insignificant
Water content	Yes. Hydraulic conductivity	Insignificant, saturation will be rapid	No	-
Gas content	No	-	Yes	Insignificant
Hydrovariables (pressure and flows)	Yes. Basic variables.	Included in the hydro-geological large scale model	Yes	Included in the hydro-geological large scale model
Stress state	No	-	No	-
Top seal materials – composition and content	Yes. Hydraulic conductivity	Model parameters	No	
Top seal porewater composition	Yes, via viscosity of water	Included in the hydro-geological large scale model	Yes	Included in the hydro-geological large scale model
Structural and stray materials	No	-	No	-

Natural analogues/observations in nature

Not required since the process is well known.

Time perspective

The hydraulic gradient that exists after closure of the repository when water saturation and pore pressure equilibrium have been established in the top seal will be adapted to the groundwater situation in the area and will remain so for the lifetime of the repository.

Handling in the safety assessment SR-Site

Included in the hydrogeological large scale model as a feature with high hydraulic conductivity, see Geosphere Process Report /SKB 2010i/.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

See Section 7.2.1 Water transport under unsaturated conditions.

7.2.3 Gas transport/dissolution

Overview/general description

Gas transport in the top seal is basically the same process as that in the central area, see Section 6.2.3. However, since the conductivity of the material will be high, trapped gas will escape very easily and the process can be neglected in the assessment.

Handling in the safety assessment SR-Site

The process is neglected and the saturation of the top seal is assumed to be rapid, see also Section 7.2.1.

7.2.4 Piping/erosion

Overview/General description

Water inflow into the top seal will take place mainly through fractures and will contribute to the wetting of the crushed rock. However, if the inflow is localised to fractures that carry more water than the crushed rock can adsorb, there will be a build-up of water pressure in the fracture and therefore an increase in the hydraulic gradient through the crushed rock. If the total pressure from the water pressure in the fracture becomes higher than the resisting total pressure the crushed rock will be deformed and an open channel or slot will be formed, where water can penetrate and continue to penetrate along the rock surface. This flow may also result in erosion of fine particles along the pipes. The processes are similar to the corresponding processes in the buffer described in Section 3.3.4.

The risk of **piping** depends on a number of factors the main ones being the following:

- The hydraulic conductivity of the crushed rock,
- The water inflow rate,
- The water pressure increase rate when water flow is stopped,
- The water inflow pattern (point wise or along a fracture).

The magnitude of **erosion** depends mainly on the grain size distribution and the percentage of fines in the crushed rock, but of course also on the flow rate.

Since the hydraulic conductivity of the blasted and crushed rock in the top seal is so high, there will be no resistance to water inflow, not even when the crushed rock is dry. This means that all inflowing water is easily absorbed by the crushed rock and that piping cannot take place. Since there are no fine-grained particles in the filling, no or little erosion will take place. If erosion of any small amount of fines would occur it would not affect the properties in any significant way.

Handling in the safety assessment SR-Site

Since piping and erosion cannot take place in the top sealing, this process is neglected.

7.3 Mechanical processes

7.3.1 Swelling/mass redistribution

This section includes all mechanical processes in the blasted and crushed rock in the top seal except liquefaction.

Overview/General description

The crushed rock has no swelling potential so it will mechanically only have passive roles. The interaction with the other parts will be governed by the stiffness, the friction angle and the own weight of the crushed rock.

In the top seal of the ramp the effective vertical stress (= total stress minus porewater pressure) varies from zero at the roof to 50-100 kPa in the floor, depending on the height of the rooms. In the top seal of the shaft, the stresses in the bottom of the top seal can be rather high due to the large depth (200 m), but the friction against the rock walls reduces the stresses significantly (silo effect). The horizontal stress is about half the vertical one.

In order to avoid that particles from the top seal penetrate into the pellets filling in the backfill below the top seal during installation there has to be a separating layer between these two parts, e.g. a concrete layer.

The backfill and the top seal of the shaft will have a complicated interaction with the clay backfill in the lower part during the filling due to the increase in vertical stress. Additional creep settlements may occur also afterwards especially due to influence of weathering (e.g. from freezing and thawing).

The **compressibility** (or stiffness) of the material can be expressed with the compression modulus according to Equation 7-1.

$$M = \Delta\sigma / \Delta\varepsilon \quad (7-1)$$

where

M = compression modulus

σ = uniaxial stress with no lateral strain

ε = uniaxial strain with no lateral strain

The **friction angle** is also very high.

The compression modulus and the friction angle depend on the grain size distribution, the shape of the grains and especially the dry density. Larger particles, more uneven shaped particles and higher dry density yield higher compression modulus and higher friction angle. All these three factors will probably be larger for the blasted and crushed rock in the top seal than for the crushed rock in the underlying parts (except maybe the density if the filling of the top seal is not compacted).

The compression modulus can be determined with oedometer tests on the actual crushed rock and the friction angle can be determined with triaxial tests or shear tests. However, such tests have not been done since it requires very large apparatuses (~1 m in diameter) due to the large particle size. It is probably not necessary to do such tests since the compression modulus and the friction angle are expected to be higher than for the underlying crushed rock and by using the same parameters the rough calculations are on the safe side.

Dependencies between process and top seal variables

Table 7-4 summarises how the process influences and is influenced by all top seal variables and how these effects are treated in SR-Site.

Interaction crushed rock in the top seal / atmosphere

If the top seal ends without any additional seal the blasted rock blocks applied in the upper part of the ramp and shaft will be in direct contact with the atmosphere and there will be no mechanical influence but human actions and ice age effects.

Table 7-4. Direct dependencies between the process “Mass redistribution” and the defined top seal variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Top seal geometry	Yes influences indirectly the stresses	Simplified calculations	No	-
Top seal pore geometry	Yes. Determines the density, which is important for the compressibility	Simplified calculations	Yes affects the density	Simplified calculations
Temperature	Insignificantly	No	No	-
Water content	Yes via density	See pore geometry	Insignificantly	No
Gas content	Insignificantly	No	No	-
Hydrovariables (pressure and flows)	Insignificantly	No	No	
Stress state	Yes. Basic variable for mechanical processes	Simplified calculations	Yes.	Simplified calculations
Top seal materials – composition and content	Yes. Determines stiffness and friction angle	Simplified calculations	No	
Top seal porewater composition	No	-	No	-
Structural and stray materials	No	-	No	-

Interaction crushed rock in the top seal/ near field rock

The following mechanical interactions between the near field rock and the backfill of crushed rock have been identified.

1. The lateral stress from the own weight of the crushed rock on the rock surface of the shaft and ramp. This stress will increase with depth especially in the shaft. It may keep loosened rock pieces in place and stabilise the rock wall.
2. Friction between the filling material and the rock surface especially in the shaft.
3. Stresses from detached rock pieces. Such pieces can affect the filling if they fall from the roof in the ramp.
4. Convergence of the rock walls. This process compresses the crushed rock in the top seal and improves the properties
5. Thermo-mechanical effects from heating and cooling the rock. The cooling phase will cause a small expansion of the open spaces and thus decrease the lateral stress from the top seal on the rock walls, but the effect is very small since the temperature changes are small in these parts.
6. Rock displacements from earth quakes or rock creep will locally affect the top seal

Interaction crushed rock in the top seal / underlying backfill

The pressure from the top seal on the underlying backfill will compress the underlying backfill, especially in the shaft, since the interface layer will probably not be able to carry the entire load. The stress increase, compression of the backfill blocks in the lower part of the ramp and shaft and probable crushing of them and resulting displacement of the interface will take place immediately at placement and thus end when the filling is completed. This means that there will probably be movements of the interface during filling. The movements will probably take place by jerks since the friction against the walls must be exceeded before there is a movement. After completed water saturation of the underlying backfill there will be a new equilibrium based on the swelling pressure and compression properties of the backfill.

Boundary conditions

The top seal has three main boundaries, namely the underlying clay backfill, the rock and the atmosphere.

Model studies/experimental studies

No such studies have been done or are foreseen to be required.

Time perspective

Compression of the underlying backfill and simultaneous own compression of the top seal material will take place immediately.

In the long-time perspective, there is a (probably negligible) creep settlement of the crushed rock backfill in the top seal and there may be local breakage of the near field rock that is caused by high stresses, excavation damages and creep in the rock.

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. There are though some experiences from backfilling of mines and other types of fillings with blasted rock stones.

Handling in the safety assessment SR-Site

Most of the mechanical effects related to mass redistribution are so small that they can be ignored in the safety assessment since the demands on the backfill of the top seal are only to preserve the seal and obstruct human intrusion.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

The mechanical properties of crushed rock fillings are well known and demonstrated in numerous examples. See also /Pusch 2009/.

Uncertainties

Uncertainties in mechanistic understanding

The mechanisms of mechanical processes in crushed rock are known well enough.

Model simplification uncertainties in SR-Site

No model will be used.

Input data and data uncertainties in SR-Site

No model will be used.

7.3.2 Liquefaction

Overview/General description

Liquefaction is a process implying that a stiff material (soil) turns into liquid due to an impact with short duration, see e.g. /Lambe and Whitman 1969/. It may take place in a loose sand when the porewater pressure is increased either due to a vibration that makes the sand particles float in the porewater (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 backfill with large stones or crushed rock.

Handling in the safety assessment SR-Site

Since the process cannot occur in the top seal, it is neglected.

7.4 Chemical Processes

7.4.1 Advective transport of species

Overview/general description

In this context, advection refers to transport of any forms of additional matter, e.g. ions, molecules or colloids, with porewater flow. The transport direction is thereby principally from volumes of high water pressure to volumes of lower pressure. The process leads to redistribution of solutes in the porewater and thus affects the porewater composition. Advection is closely related to water flow in the top seal, which is described in Section 7.2.2.

The backfill material in the top seal consists of moraine, crushed rock and rock-like material. The hydraulic conductivity is not known but can be assumed to be high (~0.1 m/s). Advective flow will thereby be the dominant transport process in this component.

Dependencies between process and top seal variables

Table 7-5 summarises how the process influences and is influenced by all top seal variables and how these effects are treated in SR-Site.

Boundary conditions

Interaction with the rock: The water transport caused by the water pressure gradients in the rock fractures is dominated by the large fractures and fracture zones.

Interaction with the atmosphere: The upper part of the top seal will connect and adapt to the groundwater system in the biosphere.

Interaction with the backfill underlying the top seal: There will be a hydraulic contact between these parts.

Model studies/experimental studies

No studies of these kinds have been performed but there is a solid knowledge of the hydraulic behaviour of fillings with crushed or blasted rock.

Natural analogues/observations in nature

Not required since the process is well known.

Time perspective

The hydraulic gradient that exists after closure of the repository when water saturation and pore pressure equilibrium have been established in the top seal will be adapted to the groundwater situation in the area and will remain so for the lifetime of the repository.

Table 7-5. Direct dependencies between the process “Advective transport of species” and the defined top seal variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Top seal geometry	Yes, major impact		No	
Top seal pore geometry	Yes, indirectly through the hydraulic conductivity. Unfilled tunnel with gaps in e.g. roof will increase the transport capacity		Indirectly, dissolution and precipitation reactions may increase or reduce the porosity, respectively.	Neglected
Temperature	Indirectly through temperature induced gradients and hydraulic conductivity. Freezing is of major importance		No	
Water content	Yes, by definition		No	
Gas content	Yes, dissolved gas is transported with flow. Indirectly through flow properties due to gas pressure, gas dissolution and precipitation.		Yes, dissolved gas transported away	Neglected
Hydrovariables (pressure and flows)	Yes, by definition		Yes, density effects may induce flow	Neglected
Stress state	No, or insignificant		No, insignificant	
Top seal – composition and content	Yes, indirectly through sorption, precipitation and dissolution reactions		Yes, indirectly through sorption, precipitation and dissolution reactions	Neglected
Top seal porewater composition	Yes, by definition		Yes, by definition	Neglected
Structural and stray materials	Yes, indirectly through dissolution of concrete, reinforcement etc.		Yes, indirectly through deterioration of the materials	Neglected

Handling in the safety assessment SR-Site

The top seal is included in the hydrogeological large scale model as a feature with high hydraulic conductivity, see the Geosphere Process Report /SKB 2010i/. This model provides the evolution of the salinity field, but also data on the transport and mixing of water types.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

See Section 7.2.1 Water transport under unsaturated conditions.

7.4.2 Diffusive transport of species

Overview/general description

A basic description of this process in the central area is given in Section 6.4.2 and in the buffer in Section 3.5.3. Because of the hydraulic situation in the top seal, diffusion is of no importance in this system part.

Handling in the safety assessment SR-Site

The process is neglected since advective transport will dominate in the top seal.

7.4.3 Sorption (including exchange of major ions)

Overview/general description

Radionuclides and major ions contained in water in the top seal can be bound to the surfaces of the large rocks in the same way as has already been described for the crushed rock material of the central area, (Section 6.4.3). In a qualitative sense, the sorption processes will be nearly identical to those taking place in crushed rock material, although the proportion of the various types of mineral surfaces is likely to differ somewhat between crushed vs. non-crushed material. Quantitatively, sorption onto large rock blocks will be of comparatively little importance, due to their small specific surface area and the comparatively short contact time of percolating water.

Dependencies between process and top seal variables

Table 7-6 shows how the process influences and is influenced by all top seal variables.

Table 7-6. Direct dependencies between the process “Sorption” and the defined top seal variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence? (How/why not)	Influence present? (Yes/No) Description	Handling of influence? (How/why not)
Top seal geometry	No		No	
Top seal pore geometry	No (not on macroscopic scale)		No	
Temperature	Yes	Influence of temperature on sorption must be acknowledged, but effect is not clear. Sorption is neglected.	No	
Water content	Yes (quantitative effect of solid/water ratio would be included in K_d).	Sorption is neglected	No	
Gas content	In case of reactive gases: indirectly through porewater composition	Sorption is neglected	No	
Hydrovariables (pressure and flows)	Possibly indirectly through porewater composition	Sorption is neglected	No	
Stress state	No		No	
Top seal materials – composition and content	Yes	Sorption is neglected	Surface composition	Effect neglected
Top seal porewater composition	Yes	Sorption is neglected	Yes	See chapter on alteration (Section 7.4.4); radionuclide concentration and release are calculated
Structural and stray materials	Yes	Sorption on stray materials is conservatively excluded in SR-Site	Possibly indirectly through porewater composition/mineral equilibria	See chapter on (Section 7.4.4); radionuclide concentration and release are calculated

Influence on top seal variables: No notable influence on top seal variables is expected.

Boundary conditions

There are no particular boundary conditions to discuss for this process.

Model studies/experimental studies

There are no particular issues to discuss for this process. The basic relations are given in Sections 3.5.5 and 6.4.3.

Time perspective

In case of relatively short contact times of percolating water, it is expected that sorption, including ion exchange of major components, may not reach equilibrium. Thus, the contribution of these reactions to the mineralisation of the percolating water will also be limited.

Natural analogues/observations in nature

Surface reactions/weathering of the large rock blocks in the top seal will be similar to what is observed for large blocks of rocks in nature. I.e. their contribution of dissolved constituents to water will be limited, and the rate of weathering with respect to their overall mass will be very slow.

Handling in the safety assessment SR-Site

The process is neglected.

Uncertainties

There are no relevant uncertainties.

7.4.4 Alteration of concrete components

Overview/general description

In the top seal, cement-bearing materials can be present as construction concrete, and grout will remain in the system after backfilling this system part. The alteration of such materials can affect the system in two different ways: 1) as a consequence of its degradation the porosity can increase, thus creating favourable pathways for groundwater to enter into the system, and 2) the increase of alkalinity due to the interaction of groundwater with these materials could possibly enhance the dissolution rate of montmorillonite in the buffer and backfill (Section 4.4.7 in the Backfill chapter and Section 3.5.9 in the Buffer chapter), weakening the effectiveness of bentonite in buffer and the clay backfill in the deposition tunnels and in the lower part of the ramp and shaft as a hydraulic barrier.

The processes associated to the alteration of concrete components are equivalent to those considered for concrete in the tunnel plug (Section 5.4.4)

Handling in the safety assessment SR-Site

The process is neglected since:

1. The concrete used is supposed to be of low pH type,
2. There is a long distance from concrete structures in the top seal to the clay components in the deposition tunnel backfill and the buffer and the performance requirements on the clay backfill in the ramp and shaft is limited.

See also Section 5.4.4.

7.4.5 Aqueous speciation and reactions

Overview/general description

This process is in general the same as the corresponding process in the buffer (Section 3.5.7.)

Handling in the safety assessment SR-Site

No geochemical processes are considered in the top seal because of the distance to, and thus limited impact on, essential repository barriers.

7.4.6 Colloid release

Overview/general description

Fractures intersecting the top seal mean that rigid volume restrictions are not present everywhere, and that small sized material may enter the fractures. Separation of individual particles from the introduced material may then take place (dispersion).

The behaviour of the particles will be dominated by thermal motion if the particles are small enough 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 fractures.

The process is considered not relevant for the upper part (100 m) of the top seal component, since the coarse gravel material in principle has the same properties as the surrounding rock with respect to colloid release. The lower part of the top seal component (100–200 m below surface) consists of crushed rock with a fuller size distribution. The smallest fractions may in principle form colloids at the groundwater interface.

Handling in the safety assessment SR-Site

This process is neglected in the top seal due to the very small possible effect, also for the unlikely case that all particles of colloidal size are transported away.

7.4.7 Steel corrosion

Overview/general description

Steel in the reinforcements in the top seal will not be stable under repository conditions, see Corrosion of steel in the Fuel and Canister Process Report /SKB 2010k/. However, there are no long term performance requirements on the reinforcements and the corrosion products and gases are not expected to have any impact on the other parts of the repository.

Handling in the safety assessment SR-Site

The process is neglected based on the reasoning above.

7.4.8 Microbial processes

Overview/general description

Microbial processes in a crushed rock environment is described in the section about the central area (Section 6.4.9)

Handling in the safety assessment SR-Site

It is not foreseen that microbial processes can interfere with the top seal in a way that will influence the performance of the repository. The process is therefore neglected.

7.4.9 Radiation induced transformation

Overview/general description

The top seal is too far away from the canisters to be affected by the α -radiation. The effect of α -radiation from radionuclides from damaged canisters can also be neglected, since the levels will be extremely small (see Section 3.5.12).

Handling in the safety assessment SR-Site

The process is neglected.

7.5 Radionuclide transport processes

7.5.1 Speciation of radionuclides

Overview/general description

See corresponding process description for the buffer, Section 3.6.1.

Handling in the safety assessment SR-Site

This process is indirectly handled through the selection of parameters for radionuclide transport in the rock. In general, the handling of the process is the same as for the corresponding process in the geosphere, see the process Transport of radionuclides in the water phase in the Geosphere Process Report /SKB 2010i/.

7.5.2 Transport of radionuclides in the water phase

Overview/general description

The top seal can be considered as a part of the rock with high hydraulic conductivity and a high porosity. If radionuclides would enter the central area the additional transport time to the surface would be rather limited.

Handling in the safety assessment SR-Site

The top seal is considered to be a part of the rock in the radionuclide transport calculations, see the process Transport of radionuclides in the water phase in the Geosphere Process Report /SKB 2010i/.

8 Processes in the bottom plate

8.1 Thermal processes

8.1.1 Heat transport

Overview/general description

The concrete part of the bottom plate will have thermal properties similar to those of the rock and will have a very modest influence on the temperature, whereas the copper plate will contribute to distribute the heat below the buffer horizontally. Figure 8-1 shows the temperature field in the bottom region with and without account of the copper bottom plate. The concrete part is ignored. The effect of the 20 mm copper plate below the bentonite barrier will be to even out the temperature such that the central parts and the peripheral parts both tend to approach the area average. In addition, there will be a small general increase of the vertical heat flux across the bottom bentonite block, leading to a small reduction (approximately 0.2°C, cf. Figure 8-1 of the canister temperature).

Dependencies between process and bottom plate variables

Table 8-1 shows how the process influences and is influenced by all bottom plate variables.

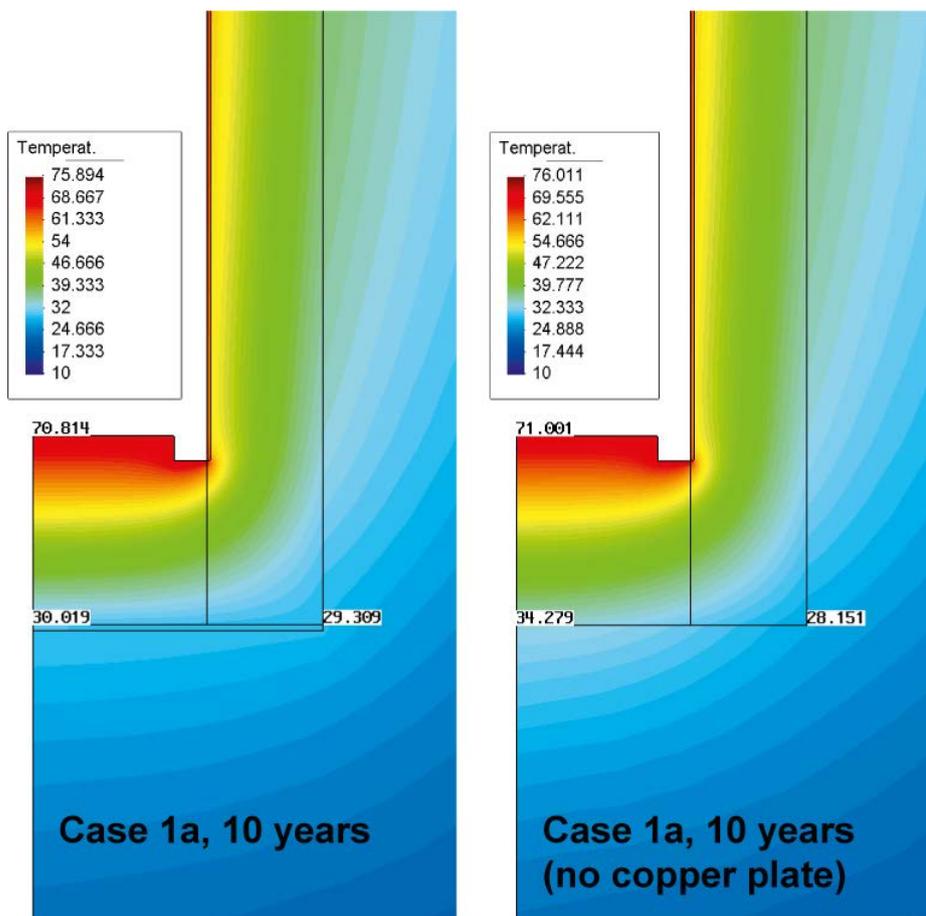


Figure 8-1. Comparison between temperatures in deposition holes with (left) and without (right) copper bottom plate. The results shown here include a 10°C in-situ temperature as a typical value of the undisturbed initial background temperature at repository depth, but not the temperature contribution from other canisters. From /Hökmark et al. 2009/.

Table 8-1. Direct dependencies between the process “Heat transport” and the defined bottom plate variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Bottom plate geometry	Yes	Copper plate geometry accounted for in thermal near-field models	Indirectly via temperature	Ignored
Bottom plate pore geometry	Yes	Ignored	Indirectly via temperature	Ignored
Temperature	Yes. Heat transport is slightly temperature dependent.	Ignored	Yes. By definition	Result of near-field thermal model.
Bottom plate water content	Yes. Thermal conductivity of the concrete foundation depends on water content	Ignored	Indirectly via temperature. High temperatures and high temperature gradients may dehydrate concrete foundation (or delay saturation)	Ignored
Bottom plate gas content	Indirectly via water content	Ignored	Indirectly via water content	Ignored
Hydrovariables (pressure and flows)	No		Indirectly via temperature	Ignored
Stress state	No		Indirectly via temperature	Ignored
Bottom plate materials – composition and content	Yes. Composition affects thermal conductivity	Copper plate included in model	Possibly via temperature	Ignored
Bottom plate porewater composition	Possibly via temperature	Ignored	Possibly via temperature	Ignored

Bottom plate geometry: The geometry of the bottom plate, i.e. the copper plate thickness and the concrete foundation thickness control the way the bottom plate influences the heat dissipation from the lower parts of the deposition hole. The temperature increase will give a modest volume expansion. If the thermally induced stresses lead to fracturing of the concrete foundation there could be some additional, but modest, volume expansion because of dilation (see text below under “bottom plate pore geometry”).

Bottom plate pore geometry: The copper plate does not have any pore system. The thermal conductivity of the concrete foundation varies with the void ratio, as it does for all porous materials and similar to the way it varies with the void ratio of the backfill in the deposition tunnels. The pore geometry could potentially be affected by thermally induced crack formation, i.e. corresponding to the way spalling may affect the porosity in the walls of the deposition holes. The uniaxial compressive strength of concrete ranges between 10 and 60 MPa depending on composition /Boverket 2004/. The thermally induced stresses in the bottom plate region are about 30 MPa at the time of the peak stress (assuming the thermo-elastic properties to be similar to those of the rock) /Hökmark et al. 2010/. For typical concrete materials, the expansion coefficient is some 50-100% higher than for the rock types found at the sites, while the E-modulus is in the range of 20-40 MPa, i.e. some 30-60% of typical rock type moduli /Ingelstam et al. 1971/. This means that the stress estimate above is reasonably valid and that the stress in the concrete foundation may approach or exceed the concrete uniaxial strength. For dry deposition holes where the vertical support pressure is limited by the weight of the canister/buffer system, this may lead to fracture initiation and possibly fracturing with an associated change in porosity and pore geometry. The fracturing cannot be expected to be extensive; a modest amount of inelastic deformation will release the stresses, that just marginally exceed the strength, sufficiently that the stability is restored. The change in porosity and pore geometry will have some impact on the permeability of the concrete plate (see text under “hydrovariables”).

Temperature: Heat transport influences the temperature by definition. There is probably a small temperature dependence in the heat transport properties of the concrete foundation (as there is for rock). The volume fraction of the near-field taken up by the bottom plate is too small to have any significant influence on the thermal evolution in the interior of the deposition hole (cf. Figure 8-1). The copper plate is nevertheless explicitly included in the thermal near-field models.

Water content: The heat transport will not affect the water content, other than indirectly via the temperature. The conductivity-saturation relations that apply for the buffer and the deposition tunnel backfill are, in principle, valid also for the concrete foundation. Because of the small volume taken up by the bottom plate, water content-induced conductivity variations are not important to the thermal evolution in the interior of the deposition hole.

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, i.e. they are of no importance.

Hydro variables: The heat transport in the bottom plate has a very small influence on its own temperature and consequently insignificant influence on the hydro variables. The raised temperature and the following thermal strain may generate some fracturing of the concrete foundation that could increase the permeability (see text above under “pore geometry”). The small volume of the concrete foundation and the way it is hydraulically separated by the copper plate from the buffer means that possible permeability changes caused by the temperature increase can be ignored. Similar as for the rock, effects of water flow on the heat transport can be neglected.

Stress state: The elevated temperatures will affect the stresses. Depending on the thermal volume expansion of the concrete foundation, there may be different types of stress gradients or stress concentrations. Possibly, there could be thermally induced fracturing of the concrete foundation (see text under “pore geometry” above). The stress state does not have any practically influence on the heat transport, although there may be some stress dependence on the thermal conductivity.

Bottom plate materials – composition and content: The composition of the bottom plate will influence the thermal conductivity. Relevant conductivity estimates are made in the near-field models /Hökmark et al. 2009/.

Bottom plate porewater composition: The copper plate does not contain any porewater. The composition of the small amounts of water contained in the pores of concrete foundation cannot have any significant influence on the heat transport properties. Temperature effects on the composition are possible, cf. handling of chemical process.

Boundary conditions

The bentonite-copper interface, the vertical rock walls and the horizontal bottom of the deposition hole are the boundaries of the bottom plate. There is a vertical heat flux on the top boundary. That flux decreases proportionally with the canister power. At the rock walls, the temperature varies slowly over time at a rate given by the canister power, the rock thermal properties and the repository layout.

Model studies/experimental studies

There are no studies that specifically address the thermal conditions in the bottom plate. The bottom plate is, however, included in near-field thermal analyses.

Natural analogues/observations in nature

Not applicable.

Time perspective

The duration of the thermal pulse generated by the decaying fuel is a few thousand years. For the bottom plate, the temporal evolution coincides with that of the buffer (cf. Section 3.2.1).

Handling in the safety assessment SR-Site

Because of the modest impact on the temperatures in the interior of the deposition hole, there is no specific handling of heat transport in the bottom plate. The copper plate is, however, explicitly included in the thermal near-field models.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

/Hökmark et al. 2009/ and /Hökmark et al. 2010/ will undergo a documented factual and quality review.

Uncertainties

Uncertainties in mechanistic understanding

There are no major uncertainties in mechanistic understanding of the heat transport itself. The concrete foundation is a system with solid, liquid and gas phases and obeys physical laws for such systems.

Model simplification uncertainties in SR-Site

Not relevant since the process is not modelled (other than by inclusion of the copper plate in the thermal near-field models)

Input data and data uncertainties in SR-Site

Not relevant since the process is not modelled (other than by inclusion of the copper plate in the thermal near-field models).

8.1.2 Freezing

Overview/general description

Freezing of the bottom plate is of no significance, since no long term performance is expected from the concrete. The same process takes place in the material around the bottom plate as described in the corresponding process description for the buffer (see Section 3.2.2). The bottom plate will not change anything in respect to freezing and thawing.

Handling in the safety assessment SR-Site

Freezing of the bottom plate is not treated in SR-Site.

8.2 Hydraulic processes

8.2.1 Water uptake and transport under unsaturated conditions

Overview/General description

The **hydro-mechanical evolution** of the bottom plate during the repository lifetime is the following.

The copper plate is installed and concrete poured into the about 15 cm thick slot between the rock surface and the copper plate. When the concrete has fully matured, the entire space is assumed to be filled. In the mean time until the bentonite buffer is emplaced, the concrete will be completely water saturated.

The buffer and canister is emplaced and, due to the bentonite protection and by draining and discharging water from the deposition hole, there is only a thermo-mechanical interaction between the bottom plate and the buffer. When the protection is removed and the slot filled with pellets, water will enter and the water uptake starts in the buffer.

At that time, a rather complicated interplay between the bottom plate, the buffer and the rock will start. Since the contact zones between the concrete and both the rock and the copper plate are not tight, water will penetrate and a water pressure will act on the plate. If this water pressure is higher than the weight of the buffer and the canister, and later also the backfill, the entire package will lift and be moved upwards. The water pressure required for this unpleasant scenario is 120–220 kPa depending on if the backfill has been placed. There are some processes that prevent or limit this scenario:

- The water pressure will spread to the pellets filling and the pellets filling cannot withstand high water pressure. Piping will instead occur, which means that at some level of the water pressure, a piping channel will occur and the water will flow out of the deposition hole
- If the backfill is placed and almost in contact with the roof, the upwards displacement is limited.
- A displacement will in itself regulate the pressure and the inflow rate must be rather high in order to maintain the pressure.

After full saturation, there will be full swelling pressure on the plate. With time, the copper plate will corrode and the concrete be dissolved and the cement dissipate. Although the ballast material is supposed to be left, there will probably be some settlement of the buffer due to the compression of these parts. There will also be a remaining very permeable zone along the entire bottom of the deposition hole.

The hydraulic processes are separated so that the saturation phase is assumed to take place before emplacement of the buffer and all the complicated hydro-mechanical processes will take place after full saturation and are handled in Section 8.2.2.

Dependencies between process and bottom plate variables

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

Table 8-2. Direct dependencies between the process “Water uptake and transport under unsaturated conditions” and the defined bottom plate variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Bottom plate geometry	Yes	Negligible	No	
Bottom plate pore geometry	Yes. Via void ratio (density) and void geometry	Negligible	No	
Temperature	Yes.	Negligible	Yes	Negligible
Bottom plate Water content	Yes. Via degree of saturation	Negligible	Yes	Negligible
Bottom plate gas content	Yes. Via the gas pressure and degree of saturation	Negligible	Yes	Negligible
Hydrovariables (pressure and flows)	Yes. Basic.	Negligible	Yes	Negligible
Stress state	No		No	
Bottom plate materials – composition and content	Yes. Hydraulic conductivity	Negligible	No	
Bottom plate porewater composition	No		No	

Boundary conditions

Interaction with the rock: The rock supplies water to saturate the concrete. Very little water is needed.

Interaction with the buffer: The plate prevents hydraulic interaction

Interaction with the radial slot that is left after installation of the bottom plate: Supplies water to saturate the concrete

Model studies/experimental studies

A similar design of the bottom plate has been used in the Prototype Repository but no information about the wetting of the concrete has been available and is not considered to be of interest.

Natural analogues/observations in nature

Not applicable.

Time perspective

Water saturation of the concrete in the bottom plate is expected to take place before the buffer is emplaced.

Handling in the safety assessment SR-Site

The water saturation of the bottom plate itself is not considered in SR-Site. However, the mechanical interaction between the buffer and the bottom plate is included in the THM-modelling, see Section 8.3.1.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

Not relevant since not handled in safety assessment

Uncertainties

Not relevant since not handled in safety assessment.

8.2.2 Water transport under saturated conditions

Overview/General description

Two main cases can be distinguished.

1. One is a high water pressure in the entire surface between the rock and the concrete that can be present rather soon after installation of the buffer.
2. The other one is the long term effect with a highly permeable zone between the rock in the bottom of the hole and the buffer material when the copper has corroded and the concrete have been disintegrated.

The hydro-mechanical evolution is described in Section 8.2.1.

Dependencies between process and bottom plate variables

Table 8-3 summarises how the process influences and is influenced by all bottom plate variables and how these effects are treated in SR-Site. The table mainly concerns the long term effect.

Table 8-3. Direct dependencies between the long term effect of the process “Water transport under saturated conditions” and the defined bottom plate variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Bottom plate geometry	Yes	Included in models	No	
Bottom plate pore geometry	Yes, after degradation	Included in the model	Yes	Washing out of cement
Temperature	Yes	Negligible	No	
Bottom plate Water content	No		No	-
Bottom plate gas content	No		No	
Hydrovariables (pressure and flows)	Yes. Basic variables.	Calculations	Yes	Calculations
Stress state	No	-	No	-
Bottom plate materials – composition and content	Yes, after degradation	Model parameters	Yes	Washing out of cement
Bottom plate porewater composition	Yes	Negligible	No	

Boundary conditions

Interaction with the rock

Case 1: Since the contact zones between the concrete and both the rock and the copper plate are not tight, water will penetrate and a water pressure will act on the plate. If this water pressure is higher than the weight of the buffer and the canister, and later also the backfill, the entire package will lift and be moved upwards. The water pressure required for this unpleasant scenario is 120–220 kPa depending on if the backfill has been emplaced. As described earlier, there are some processes that prevent or limit this scenario.

Case 2: With time the copper plate will corrode and the concrete will suffer from degradation and leaching. There will thus be a remaining very permeable zone along the entire bottom of the deposition hole.

Interaction with the buffer

After long time (case 2) there will be hydraulic contact between the permeable zone in the degraded concrete and the buffer.

Interaction with the annular slot at the rock surface that is left after installation of the bottom plate

Case 1: Water that enters from the rock surface beneath the concrete in the bottom plate will flow out to the radial slot that is filled with bentonite pellets and will speed up the water filling of the pellets in the slot. If the pellets filling has time to interact with the bentonite block and form a swelling pressure that is high enough to seal, there may be a substantial water pressure. Tests done so far have shown that the pellets filling cannot withstand high water pressure without piping, but 100–200 kPa (which is in the same order as needed for lifting the bentonite/canister package) can probably be resisted.

Case 2: After full saturation and homogenisation, the slot will be filled with bentonite with a somewhat lower density than the rest of the buffer. This slot will thus be in direct hydraulic contact with the permeable zone formed by the degrading concrete.

Model studies/experimental studies

A similar design of the bottom plate has been used in the Prototype Repository. No severe consequences of case 1 have so far been observed.

The consequences of case 2 with a permeable concrete zone will be included in the safety case model.

Natural analogues/observations in nature

Not applicable.

Time perspective

Case 1: Takes place before full saturation is reached, that is within about 100 years.

Case 2: Long time effect that must be considered for the lifetime of the repository.

Handling in the safety assessment SR-Site

Case 1 is difficult to handle. A serious investigation of this is still done. Due to the vulnerability of the bentonite pellets to piping there will probably not be any high water pressure anyway not in the beginning. With time, as the swelling pressure increases, the water pressure may be higher but then there is also strength (friction) between the rock and buffer that prevents axial displacements. However, it is a complicated scenario and it may be very difficult to prove that it does not occur.

Case 2 is included in the model for the safety assessment.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

Modelling of the two cases is reported in a general THM modelling report that will undergo a documented factual- and quality review /Åkesson et al. 2010a/.

Uncertainties

Uncertainties in mechanistic understanding

Case 1: The mechanistic understanding of this process is good but the consequences are difficult to evaluate.

Case 2: Can be modelled as a porous material, which is well known.

Model simplification uncertainty in SR-Site

Case 1: There is no good way to model this situation. Experiences and model tests are needed.

Case 2: No model simplification needed.

Input data and data uncertainty in SR-Site

Case 1: Large uncertainty in the data and the consequence. The data selection is discussed in the buffer THM Data Report /Åkesson et al. 2010b/

Case 2: The hydraulic properties are not known so a high hydraulic conductivity must be assumed. The data selection is discussed in the buffer THM Data Report /Åkesson et al. 2010b/

8.2.3 Gas transport/dissolution

Overview/general description

The bottom plate will be saturated before the deposition of the buffer and the canister. The saturation phase is therefore of no concern in the assessment (see also Section 8.2.1).

A degraded porous bottom plate could potentially act as a sink/pathway for gas release from a corroding canister insert in a defective canister. This effect would be beneficial since it would make it easier for the gas to escape. However, it will be impossible to demonstrate that this actually is the case.

Handling in the safety assessment SR-Site

The process is neglected based on the reasoning above.

8.2.4 Piping/erosion

Overview/General description

This process may not take place in the bottom plate but is of great importance in the buffer material, especially in the pellets-filled slot, for the hydraulic scenario that may occur after installation (see case 1 for the process “Water transport under saturated conditions” Section 8.2.2).

Handling in the safety assessment SR-Site

The process is not relevant for the bottom plate and is therefore not handled.

8.3 Mechanical processes

8.3.1 Swelling/mass redistribution

Overview/General description

Just as for the hydraulic processes the mechanical can be divided into two cases.

Case 1 is the same as for the hydraulic processes. A high water pressure may occur in the surface between the rock and the concrete and can be present rather soon after installation of the buffer. Since the contact zones between the concrete and both the rock and the copper plate are not tight water will penetrate and a water pressure will act on the entire plate. If this water pressure is higher than the own weight of the buffer and the canister and later also the backfill the entire package will lift and be moved upwards. The water required for this unpleasant scenario is 120-220 kPa depending on if the backfill has been placed. There are some processes that prevent or limit this scenario:

- The water pressure will spread to the pellets filling and the pellets filling cannot withstand high water pressure. Piping will instead occur, which means that at some water pressure a piping channel will occur and the water will flow out of the deposition hole
- If the backfill is placed and almost in contact with the roof the upwards displacement is limited.
- A displacement will in itself regulate the pressure and the inflow rate must be rather high in order to maintain the pressure.

Case 2 is also similar to case 2 for the hydraulic processes. After full saturation there will be full swelling pressure on the plate. With time the copper plate will corrode and the concrete will suffer from degradation and leaching. Although the ballast material is supposed to be left there will probably be some settlement of the buffer due the compression of these parts.

Table 8-4 summarises how the process influences and is influenced by all bottom plate variables and how these effects are treated in SR-Site. The table mainly concerns both cases if not otherwise stated.

Boundary conditions

Interaction with the rock

Since the rock is almost incompressible it will act as a boundary for the displacements in the bottom plate.

Table 8-4. Direct dependencies between the process “Swelling/Mass redistribution” and the defined bottom plate variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Bottom plate geometry	Yes	Included in models	Yes	Case 1: Estimation of consequences Case 2: Modelling
Bottom plate pore geometry	Case 1: No. Case 2: Yes, via compressibility	Case 2: Included in the compressibility model	Case 1: No Case 2: Yes	Case 2: Included in the compressibility model
Temperature	Yes	Negligible	Case 1: Yes if displacement takes place. Case 2: No	Neglected
Bottom plate Water content	Case 1: No Case 2: Yes via compressibility	Case 2: Modelling of consequences	Yes	Case 1: Neglected Case 2: Modelling of consequences
Bottom plate gas content	No		No	
Hydro-variables (pressure and flows)	Case 1: Yes. Basic variables. Case 2: No	Case 1: Estimation of consequences	Case 1: Yes Case 2: No	Case 1: Estimation of consequences
Stress state	Case 1: Yes. Own weight of buffer etc. Case 2: Yes, via compressibility	Case 1: Yes. Own weight of buffer etc. Case 2: Included in the compressibility model	Yes	Case 1: Included in modelling Case 2: Included in the compressibility model
Bottom plate materials – composition and content	Case 1: No. Case 2: Yes, via compressibility after degradation	Case 2: Included in the compressibility model	No	
Bottom plate pore-water composition	No		No	

Interaction with the buffer:

The contact between the plate and the buffer will move with the displacement of the plate in case 1 and with the compression of the degraded concrete in case 2.

Interaction with the annular slot at the rock surface that is left after installation of the bottom plate

Case 1: Water that enters from the rock surface beneath the concrete in the bottom plate will flow out to the radial slot that is filled with bentonite pellets and will speed up the water filling of the pellets in the slot. If the pellets filling has time to interact with the bentonite block and form a swelling pressure that is high enough to seal, there may be a substantial water pressure. Tests done so far have shown that the pellets filling cannot withstand high water pressure without piping, but a pressure of 100-200 kPa (which is in the same order as needed for lifting the bentonite/canister package) can probably be resisted.

Case 2: After full saturation and homogenisation the slot will be filled with bentonite with a somewhat lower density than the rest of the buffer. The bentonite in this slot will thus be in direct mechanical contact with the porous material formed by the degrading concrete.

Model studies/experimental studies

A similar design of the bottom plate has been used in the Prototype Repository. No severe consequences of case 1 have so far been observed.

The consequences of case 2 with a compressible porous material will be studied.

Natural analogues/observations in nature

Not applicable.

Time perspective

Case 1: Takes place before full saturation is reached, that is within about 100 years.

Case 2: Long-time effect that must be considered for the lifetime of the repository.

Handling in the safety assessment SR-Site

Case 1 is difficult to handle but an attempt to model it will be done. A serious investigation of this case will be done. Due to the vulnerability of the bentonite pellets to piping, there will probably not be any high water pressure build up, anyway not in the beginning. With time, as the swelling pressure increases, the water pressure may become higher, but then there is also strength (friction) between the rock and buffer that prevents axial displacements. However, it is a complicated scenario and it may be very difficult to prove that it does not occur.

Case 2 will be modelled.

Both cases are analysed by /Åkesson et al. 2010a/.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

Modelling of the two cases will be reported in a general THM modelling report that will undergo a documented factual- and quality review /Åkesson et al. 2010a/.

Uncertainties**Uncertainties in mechanistic understanding**

Case 1: The mechanistic understanding of this process is good but the consequences are difficult to evaluate.

Case 2: Can be modelled as a porous material, which is well known.

Model simplification uncertainty

Case 1: There is no good way to model this situation but some simplified limiting calculations will be done. Experiments and model tests might be needed.

Case 2: No model simplification needed.

Input data and data uncertainty

Case 1: Large uncertainty in the data and the consequence. This is discussed in the Buffer THM data report /Åkesson et al. 2010b/

Case 2: The mechanical properties are not known but knowing the composition of the concrete a worst case can be considered. This is discussed in the Buffer THM data report /Åkesson et al. 2010b/.

8.3.2 Liquefaction

Overview/General description

Liquefaction may only occur in the porous material after degradation of the concrete. However, since there is a high swelling pressure on the porous material liquefaction is highly unrealistic. If it anyway would occur the consequences are insignificant since the material cannot move anywhere and will afterwards be the same as before.

Handling in the safety assessment SR-Site

Since the process is highly unlikely to occur and the consequences are negligible, the process is neglected.

8.4 Chemical processes

8.4.1 Advective transport of species

Overview/general description

The general description provided for the buffer in Section 3.5.2 is applicable also for the bottom plate. Specific conditions for the bottom plate are addressed below.

No advective flow may take place through the copper plate as long as it is intact, and all flow has to take place outside the edge of the plate. The advective flow in the underlying concrete will be controlled by the hydraulic conductivity as long as the cement is intact. This retarding effect will be dramatically reduced in case of a fracture in the concrete, which can develop at any time. Neither the copper plate nor the concrete are protected by bentonite. The longevity of these components is thereby controlled by the exposure to groundwater from fractures in the vicinity. The resistance to advective flow may eventually be strongly reduced, and the bottom part of the deposition hole will be a conductive zone.

Dependencies between process and bottom plate variables

Table 8-5 summarises how the process influences and is influenced by all bottom plate variables and how these effects are treated in SR-Site.

Boundary conditions

The external boundary condition for this process is the hydraulic and concentration gradient across the bottom plate system component.

Model studies/experimental studies

No specific studies by SKB or others have examined water flow in a similar system. General studies of concrete give information of the conditions in a non degenerated concrete.

Natural analogues/observations in nature

No relevant studies available.

Time perspective

Advective flow transport in conjunction with water saturation takes place on a timescale of up to hundreds of years. Flow transport after degeneration of the cement and copper may be significant.

Table 8-5. Direct dependencies between the process “Advective transport of solutes” and the defined bottom plate variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Bottom plate geometry	Yes, no material transport will take place through an intact copper plate. The transport of material is governed by the hydraulic conductivity if the concrete is intact. Introduction of fractures or chemical deterioration may strongly increase the advective flow	Included in the model for radionuclide transport	Yes, corrosion of copper due to transport of corrodants and deterioration of concrete due to interaction with flowing groundwater	Neglected since no performance is expected from the bottom plate
Bottom plate pore geometry	Yes, main parameter for hydraulic conductivity. Introduction of fractures or chemical deterioration may strongly increase the advective flow	The hydraulic conductivity is assumed to be high. Included in the model for radionuclide transport	Yes, deterioration due to interaction with flowing groundwater	Neglected since no performance is expected from the bottom plate
Temperature	Yes, affects solubility. Indirectly through porewater viscosity	Neglected, since effect is small	Yes, but small, insignificant	Neglected
Bottom plate Water content	Yes, by definition	Assumed to be saturated	Yes, by definition	Assumed to be saturated
Bottom plate gas content	Yes, by reduction of available flow area	Neglected since bottom plate is assumed to be saturated	Yes, dissolution of gas, or release of dissolved gas	Neglected since no performance is expected from the bottom plate
Hydrovariables (pressure and flows)	Yes, by definition	Included in the model for radionuclide transport	Insignificant	
Stress state	Yes, induction of fractures and regulating fracture width	Neglected, a high hydraulic conductivity is pessimistically assumed.	No	
Bottom plate materials – composition and content	Yes, through dissolution	Neglected, a high hydraulic conductivity is pessimistically assumed.	Yes, by corrosion, introduction or reactants and removal of reaction products	Neglected since no performance is expected from the bottom plate
Bottom plate porewater composition	Yes, through dissolution	Neglected, effect is assumed to be small	Yes, by definition	Neglected since no performance is expected from the bottom plate

Handling in the safety assessment SR-Site

The bottom plate can be treated as a volume with high hydraulic conductivity in the model for radionuclide transport. In SR-Site this volume is treated the same way as “spalling” zone in the canister wall /Neretnieks et al. 2010/. This may be of importance if there is a water conductive fracture which intersects the bottom plate.

Handling of variables influencing this process:

The geometry of the bottom plate and the fracture flow is included in the model. The material properties are simplified into an assumption of “high hydraulic conductivity”.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

/Neretnieks et al. 2010/ is subjected to a peer review according to the review plan for SR-Site.

Uncertainties

Uncertainties in mechanistic understanding

It is uncertain whether the bottom plate will at all have any effect on the mass transfer in the near field. However, the treatment described in this section will always be pessimistic for the mass-transfer.

Model simplification uncertainties for the above handling in SR-Site

The model approach is further discussed in /Neretnieks et al. 2010/.

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

There is no uncertainty regarding the geometry. A pessimistic value is assumed for the hydraulic conductivity. The uncertainty regarding the flow in the rock is discussed in the Geosphere Process Report /SKB 2010i/.

8.4.2 Diffusive transport of species

Overview/general description

A description of this process is given for the buffer in Section 3.5.3. In principle, the same processes are operative in hardened, water-saturated cement paste or concrete as in clay. Briefly, solutes can be transported in stagnant porewater by diffusion, following concentration gradients. The process leads to a redistribution of dissolved porewater constituents (as well as radionuclides) in the porewater. The diffusion process is strongly coupled to nearly all chemical processes in the concrete, since it accounts for transport of reactants to and reaction products from the processes.

Diffusion in cement-based materials has not been studied as thoroughly as in clays, for example. However, diffusion can be described by the same diffusion equations as are used for clays and other porous media; these equations are described in detail in e.g. /Yu and Neretnieks 1997/. In contrast to clays, no significant electrostatic effects (and hence no diffuse double layer/Donnan potential effects on diffusion and on porewater concentrations of ions) in the pore space need to be considered.

At least in experiments, the reactive nature of hardened cement paste presents a particular challenge. Alteration reactions of the solid material occur on roughly the same timescales as diffusion processes. Such transient geochemical conditions make it impossible to interpret diffusion profiles /Jakob et al. 1999/. Therefore, diffusion needs to be measured in stable systems, e.g. using cement that has been leached to reach the portlandite-dominated phase and well pre-equilibrated water.

Dependencies between process and bottom plate variables

Table 8-6 shows how the process influences and is influenced by all system variables.

Influence on variables of bottom plates: Through transport of dissolved species to and from the concrete system, diffusion will influence the overall composition and rate of alteration.

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.

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.

Influence of composition: The diffusion properties of concrete are dependent on the porosity and pore geometry which may be influenced by the composition, such as the amount and size of aggregate material. Also, sources of Ca that may lead to the precipitation of calcite will have an important influence.

Influence of porewater composition and speciation: Different species of the same element can have different diffusivities in free water and thereby also in pores. Speciation will also influence sorption, which is taken into account in the equation for D_a .

Boundary conditions

Diffusion is only considered in the context of concrete alteration rate, not for the transfer of species to other system components. At least over longer time frames, the parameters determining diffusive transport will be significantly influenced by the composition of the adjacent porewater. Carbonate-rich water will lead to the precipitation of calcite in the concrete pore structure, further decreasing porosity. On the other hand, water that is nearly carbonate free may dissolve cement minerals to the point where advective flow would become dominating /Pfungsten and Shiotsuki 1998/.

Carbonate-rich water entering as well as alkaline solutions leaving the concrete part may lead to the precipitation of minerals at the concrete-bentonite/rock boundary. This would affect the boundary conditions for the processes responsible for transferring dissolved species to and from the concrete.

In the presence of an intact copper plate, diffusion in the direction of the buffer will not be relevant.

Table 8-6. Direct dependencies between the process “Diffusive transport of solutes” and the defined component variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence? (How/why not)	Influence present? (Yes/No) Description	Handling of influence? (How/why not)
Bottom plate geometry	Yes	Neglected since advection is assumed to dominate	No	
Concrete pore geometry	Yes	Neglected since advection is assumed to dominate	No, but indirectly through influence on porewater composition	
Temperature	Yes	Influence of temperature on diffusion in concrete must be acknowledged, but effect is not established	No	
Water content	Yes	Saturated conditions are assumed	No	
Gas content	Saturated conditions assumed	Saturated conditions are assumed	For dissolved gases such as CO ₂ , CH ₄	Neglected since advection is assumed to dominate
Hydrovariables (pressure and flows)	Yes	Neglected since advection is assumed to dominate	No	
Stress state	No, but indirectly through pore geometry		No, but indirectly through influence on porewater composition / mineral equilibria	see Section 8.4.4
Bottom plate materials – composition and content	Yes, defines magnitude of diffusivities		No, but indirectly through influence on porewater composition / mineral equilibria	see Section 8.4.4
Porewater composition	Through effect on speciation. Defines magnitude of diffusivities	Neglected since advection is assumed to dominate	Through diffusive transport of main dissolved constituents	see Section 8.4.4

Model studies/experimental studies

In the context of radionuclide migration, there is a very limited number of well-documented studies on hardened cement paste available e.g. /Jakob et al. 1999, Tits et al. 2003/. Most experiments were done with relatively inert tracers, and only a few experiments used tracers that interact significantly with the cement matrix. These studies show that experiments can only be interpreted when transient conditions (alteration during the experiment) are avoided.

There are additional studies that have been performed in the context of concrete use for construction. These are often of a more macroscopic character and/or rely on observations made on existing concrete structures. Because of its implications for steel corrosion, there is a vast amount of such literature on chloride (see e.g. /Ollivier and Nilsson 1997/ and references therein).

Time perspective

As pointed out above, the time frame of diffusion is similar to the time frame of mineral alteration.

Natural analogues/observations in nature

Observations made in recent structures and on historic concrete samples show that the composition of the contacting water, and its effect on mineral dissolution/precipitation is the key to understanding transport processes.

Handling in the safety assessment SR-Can

The process is neglected in the context of radionuclide transport, since advection is assumed to dominate. The handling of diffusion of major ions is described in Section 8.4.4 Alteration of concrete.

Uncertainties

The assumption that advection will dominate is pessimistic. However, if diffusion would dominate, the mass transfer in the bottom plate would be negligible compared to the mass transfer in the buffer itself.

8.4.3 Sorption (including exchange of major ions)

Overview/general description

For the actual copper plate (copper metal surface), no sorption reactions are expected to take place and this process is neglected.

In the concrete part of the bottom plate, radionuclides and major ions may undergo a range of interactions with the matrix (hardened cement paste). In comparison, interaction with the aggregate material can often be neglected. Exceptions to this may be sorption of simple cations, especially Cs, to layer silicate minerals contained in the aggregate material derived from crystalline rock. This process is discussed in Section 6.4.3.

The interaction of radionuclides and major ions with the cement matrix is probably best described with the term “uptake”. Because the cement matrix consists of several types of mineral phases with different properties, a range of solid-liquid interactions may take place. At the same time, the relative proportion of mineral phases as well as their properties are known to change as a function of cement matrix degradation. This process will to some degree depend on cement and groundwater composition, but is in general terms fairly well understood and the cement matrix composition can be modelled fairly well as a function of porewater exchange cycles.

In case of the more crystalline aluminates phases (ettringite/monosulphate, hydrogarnet), solid-liquid interactions may involve ion exchange and surface complexation reactions as well as the formation of classical solid solutions. However, the most relevant solid phases in hydrated cement systems are calcium-silica-hydrates (CSH), which are amorphous, very reactive, and possess a high specific surface area. Interaction of major ions, and in particular of actinides/lanthanides and transition elements, with these mineral phases typically results in some type of incorporation, often in an ill-defined and non-stoichiometric fashion. The latter case may be non- or only partly reversible.

As a result of this complexity, the nature of the uptake process has not yet been established for most radioelements. This is corroborated by the amorphous and reactive nature of cement mineral phases. Further, nearly all cements contain a relatively high inventory of stable isotopes of many potentially relevant radionuclides, which means that isotopic exchange rather than chemical interactions have to be considered in some cases.

On the other hand, a number of systematic uptake studies has become available during the last decade, which allows defining K_d for many relevant elements as a function of conditions within reasonable uncertainty ranges. As indicated in Section 5.4.3 (Sorption in tunnel plug), no adverse effects on sorption by concrete admixtures are expected. Available cement degradation models further allow tying sorption data developed for one particular cement degradation state to other relevant stages.

Interaction of the solid cement matrix with groundwater influences the overall system composition (and hence sorption of trace elements), but the nature of the respective processes are closer to dissolution/precipitation phenomena than to ion exchange in the classical sense (see Section 8.4.4 for more details).

Dependencies between process and bottom plate variables

Table 8-7 shows how the process influences and is influenced by all bottom plate variables.

Table 8-7. Direct dependencies between the process “Sorption” and the defined bottom plate variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence? (How/why not)	Influence present? (Yes/No) Description	Handling of influence? (How/why not)
Bottom plate geometry	No	RN sorption by bottom plate materials is neglected. Total mass considered for reactions with major ions	Only for concrete (leaching, sorption of Ca on secondary phases, possible changes in mechanical properties)	See Section 8.4.4
Pore geometry	No (not on macroscopic scale)		Only for concrete (leaching of Ca, possible changes in mechanical properties)	See Section 8.4.4
Temperature	Yes, influence of temperature on exchange reactions must be acknowledged, but effect is not clear	Neglected	No	
Water content of concrete	Possibly indirectly through porewater composition		No	
Gas content of concrete	In case of reactive gases: indirectly through porewater composition		No	
Hydrovariables (pressure and flows)	No		Possibly indirectly through porewater composition / mineral equilibria	
Stress state	No		No	
Composition of concrete	Yes	Radionuclide sorption is neglected	Yes	See Section 8.4.4
Concrete porewater composition	Yes	Radionuclide sorption is neglected	Yes (depending on degradation stage)	See Section 8.4.4

Influence on variables of bottom plate: As pointed out above, interaction of the solid cement matrix with groundwater influences the overall system composition. This may result in an alteration or (partial) loss of mechanical properties of the concrete part.

Influence of the composition of concrete part: The concrete will impose very alkaline conditions (pH > 11) in the immediate vicinity, irrespective of small variations in its composition. As pH is one of the main parameters influencing sorption, the solid-liquid distribution of trace and major elements in the affected areas will be affected as well. In the concrete part of the bottom plate itself, radionuclide sorption is neglected.

Influence of temperature: As pointed out in Section 3.5.5, not enough data as a function of temperature are available to clearly evaluate temperature effects. This is also true for cementitious materials. While an increase or decrease of the temperature (in comparison to room temperature) is potentially of importance for uptake, it will most likely have a more pronounced effect by directly affecting the mineralogy of the cement matrix.

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 porewater in the concrete material and the water in its adjacent components, i.e. mainly the boundary conditions of the process advection.

Model studies/experimental studies

A vast amount of experimental as well as a number of modelling studies is available regarding the uptake of various radionuclides by hardened cement paste, individual cement mineral phases (CSH, etc.), as well as whole concrete and mortar samples. According to a fairly recent analysis of the state of the art /ANDRA 2005/, the uptake mechanism is in many cases not established yet, but the available database has become sufficiently systematic to define K_d for many elements, especially for the portlandite-dominated state. Some systematic datasets as well as some model approaches can be used to relate such values to other degradation states. Since radionuclide sorption in the concrete part of the bottom plate is neglected, no further discussion of these topics is given here. For a discussion of degradation processes and stages, see Section 8.4.4.

Time perspective

Uptake processes are in many cases initially completed within weeks, followed by a much slower process that may extend over the timescale of years. Available evidence /Ziegler 2000, Ochs et al. 2003/ suggests that the first process represents some type of (near)-surface attachment, whereas the latter is related to further diffusion into particles, incorporation, etc. Especially after long time frames of interaction, uptake is likely to be only partly reversible.

Natural analogues/observations in nature

Because cement is a technical product, only few (natural) analogues exist. Best studied is the Marqarin site; the respective research activities and results are extensively documented (see /Smellie 1998/ and references therein). Because of the reactivity of hydrated cement mineral phases, it is generally difficult to deduce the original uptake process on the basis of aged samples, however.

Handling in the safety assessment SR-Site

Radionuclide sorption on the bottom plate is neglected. For handling of possible effects of concrete alteration, see Section 8.4.4.

Uncertainties

As pointed out above, the mechanisms of uptake are still not established for many cases. As the process of radionuclide sorption is neglected, no uncertainties regarding handling need to be discussed. For a discussion of uncertainties related to concrete alteration, see Section 8.4.4.

8.4.4 Alteration of concrete

Overview/general description

This process is in general identical with the corresponding alteration process for concrete in the tunnel plug (Section 5.4.4)

Handling in the safety assessment SR-Site

The alteration process for the bottom plate is assumed to be comparable with the same process for the tunnel plug, Section 5.4.4. Only the effect on the geochemistry is studied. The hydraulic properties of the bottom plate are always assumed to be “degraded”.

8.4.5 Aqueous speciation and reactions

Overview/general description

This process is in general the same as the corresponding process in the buffer (see Section 3.5.7)

Handling in the safety assessment SR-Site

The process is included in a separate modelling task of the concrete degradation. This is further described in the section for the plug (Section 5.4.4).

8.4.6 Corrosion of copper

Overview/general description

The copper plate will behave similar to the copper in the canister overpack, see Fuel and Canister Process Report /SKB 2010k/, section copper corrosion. The difference is that the copper plate only has bentonite on one side and the other side will be exposed to the concrete part of the plate.

Handling in the safety assessment SR-Site

The copper plate is neglected in SR-Site. It is assumed to have no mass-transfer resistance in the assessment.

8.4.7 Microbial processes

Overview/general description

Microbial processes are stimulated by organic compounds and the gases hydrogen and methane /Madigan et al. 2008/. The addition of organic compounds to low pH cement, such as polycarboxylate polymers, may support microbial growth and activity in cases where the added compounds dissolve, or never solidifies. The peripheral slot volume, 30 mm wide, where the concrete, the copper plate, the buffer and the rock meet may be beneficial for microbial growth and activity, if water is available and the buffer does not reach full swelling pressure in this position. The microorganisms can then obtain energy and nutrients for growth from both the buffer material and the concrete. The higher pH of the concrete to be used (<11), relative to groundwater, is not a conceptual problem for microorganisms as they have been found active at pH above 12 /Pedersen et al. 2004/. Microbial growth on concrete additions may result in production of sulphide, acid, gas and complexing agents as briefly outlined next. Sulphide production may occur if organic concrete additions dissolve and sulphate is available. If sulphide production occurs in the interfaces of concrete and other structures during the aerobic swelling phase, sulphuric acid may form by the spontaneous oxidation of sulphide with oxygen. Sulphide production may also be a problem for the copper plate as sulphide is corrosive to copper. Production of methane may occur if low molecular carbon compounds such as formaldehyde are added to and subsequently leached from the concrete. Bacteria form complexing agents /Johnsson et al. 2006, Essén et al. 2007, Moll et al. 2008/ during growth. Such agents may produce if organic concrete additions become available to microbial processes.

Dependencies between process and bottom plate variables

Table 8-8 shows how the process influences and is influenced by all bottom plate variables.

Table 8-8. Direct dependencies between the process “Microbial processes” and the defined bottom plate variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Bottom plate geometry	No		No	
Concrete pore geometry	No		No	
Temperature	Yes, microbial activity increases with temperature	This effect is not considered in SR-Site	No	
Hydro-variables (pressures & flows)	Yes, water is needed for growth of micro-organisms. Microbes grow on hydrogen and methane. Pressure is not important	This effect is not considered in SR-Site	Yes, microbes may form methane and hydrogen	Limited growth is assumed due to low availability of water and nutrients
Water content	Yes, availability of water	Saturated conditions assumed	No	
Gas content	Indirectly through water content		No	
Stress state	No		No	
Materials – composition and content	Yes, if concrete is added with substances that dissolve and support microbial activity	Limited growth is assumed due to low availability of water and nutrients	Yes, if acids are produced from degradation of concrete additions	Limited growth is assumed due to low availability of water and nutrients
Porewater composition and content	Yes, if dissolved organic components are present, microbes can grow	Limited growth is assumed due to low availability of water and nutrients	Yes, decomposition of organic dissolved components may occur, pH may be influenced	Limited growth is assumed due to low availability of water and nutrients

Boundary conditions

The boundary condition for the process is the amount of dissolved organic compounds from the low pH cement and the bentonite at the interface between the copper plate, concrete, rock and buffer.

Model studies/experimental studies

Not available.

Natural analogues/observations in nature

Growth and activity of microbes have been observed at pH above 12 /Pedersen et al. 2004/.

Time perspective

Microbial processes will start when water is available. The process rates will probably be largest in the peripheral slot with interfaces between buffer, the copper plate, rock and concrete during a wet oxygenic stage, before full swelling and reducing conditions occur.

Handling in the safety assessment SR-Site

In the treatment of the geochemical evolution in the bottom plate, microbial reactions need to be considered. Production of sulphide in the bottom plate will be considered in the assessment of canister corrosion.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

All the references in this section are from peer reviewed scientific journals. However, the most recent ones may be in the progress of being published.

Uncertainties

The key uncertainty is the presence and availability of nutrients. This can be handled by a sensitivity study.

Uncertainties in mechanistic understanding

The amount of dissolving organic concrete additions to the porewater and the peripheral slot environment is unknown.

Model simplification uncertainty in SR-Site

Not relevant since no model for microbial processes in contact with low pH cement is used.

Input data and data uncertainty in SR-Site

Not relevant since no model for microbial processes in contact with low pH cement is used.

8.5 Radionuclide transport processes

8.5.1 Speciation of radionuclides

Overview/general description

See corresponding process description for the buffer, Section 3.6.1

Handling in the safety assessment SR-Site

This process is indirectly handled through the selection of parameters for radionuclide transport in the buffer. In general, the handling of the process is the same as for the corresponding process in the buffer (see Section 3.6.1).

8.5.2 Transport of radionuclides in the water phase

Overview/general description

As long as the copper plate is intact there will be no transport of radionuclides in or through the bottom plate. However, the copper is not protected by a bentonite barrier and can be exposed to corrosion from species in the groundwater. This is especially the case when the bottom plate is in contact with a water-carrying fracture and the concrete is degraded (see also Section 3.6.2).

If the copper is corroded and the concrete is degraded the bottom plate may act as a porous media with a rather high hydraulic conductivity. This means that the bottom plate could act as a sink for radionuclides and as a source for canister corrodants.

Dependencies between process and bottom plate variables

Table 8-9 summarises how the process influences and is influenced by all component variables and how these effects are treated in SR-Site.

Table 8-9. Direct dependencies between the process “Transport of radionuclides in the water phase” and the defined component variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Copper plate geometry	Yes, determines if radionuclide transport can occur	Neglected, a limited lifetime for the copper plate can be assumed in radionuclide transport calculations	No, the process has no relevance for the copper plate	
Concrete geometry	Yes, gives the actual size of the potential sink	Included as a volume in radionuclide transport calculations	No	
Concrete pore geometry	Yes, determines the porosity	Included as a porosity in radionuclide transport calculations	No,	
Temperature	Yes	Neglected, since the effect of the temperature on the radionuclide transport is very minor	No	
Water content	Yes	Assumed to be saturated when radionuclide transport occurs	No	
Gas content	Yes	Assumed to be saturated when radionuclide transport occurs	No	
Hydrovariables (pressure and flow)	Yes	The water flow is included in the radionuclide transport calculations	No	
Stress state	No		No	
Concrete composition	No, assumed to be degraded when radionuclide transport occurs		No	
Concrete porewater composition	Yes	Neglected, since the effect of the sorption in the degraded concrete is conservatively neglected	Yes	Output from radionuclide transport calculations

Boundary conditions

The inner boundary for this process is the concentration profile of radionuclides in the buffer. The outer boundary is the water in rock, especially if a fracture intersects the bottom plate.

Model studies/experimental studies

In general, this process represents diffusion of radionuclides from bentonite into a porous volume. This is described for the buffer in Section 3.5.3.

However, no studies that directly assess this particular process have been performed.

Natural analogues/observations in nature

Not relevant

Time perspective

This process may be active all timescales after canister failure.

Handling in the safety assessment SR-Site

Radionuclide transport in the buffer is handled in the integrated modelling of radionuclide transport for the repository as described in Section 3.6.1. The bottom plate will be included as an element in the COMPULINK integrated near field model, see the SR-Site Model summary report /SKB 2010n/. The conceptual and mathematical model is described in /Neretnieks et al. 2010/, see also Section 8.4.1.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

The SR-Site Model summary report /SKB 2010i/ and /Neretnieks et al. 2010/ will be subjected to a documented factual- and quality review according the SR-Site standards.

Uncertainties

See Section 8.4.1.

9 Processes in borehole seals

9.1 Thermal processes

9.1.1 Heat transport

Overview/general description

For borehole seals extending a distance $l = 400$ m from the repository horizon to the ground surface, the heat flow Q would be less than 0.2 W if the temperature difference DT between the ends of the tube is about 40°C even if the seals are made of solid 75 mm ($A = 0.0044\text{m}^2$) diameter copper rods with thermal conductivity $\lambda = 390$ W/(m·K). ($Q = \lambda * A * DT / l$). In reality it will be much less.

Because of the small heat flow, the temperature disturbances (cooling of rock in the bottom end and heating in the top end) will be very modest and involve very small rock volumes in the immediate vicinity of the tube. In the concrete portions and, in particular, in the bentonite filling not covered by copper tubes, the heat flow is vanishingly small. The temperatures of the borehole seals are almost completely determined by the thermal evolution of the surrounding rock, i.e. practically independent of the heat transport within the seals.

Handling in the safety assessment SR-Site

The evolution of the rock temperature at different positions within and around the repository is calculated in /Hökmark et al. 2009/. Because of the small thermal gradients and the relatively low temperatures in the borehole seals, there is no specific handling of the heat transport process in the borehole seals.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

The gradient and temperature statements are supported by results obtained using calculation schemes described in /Claesson and Probert 1996/. While this particular report is not peer or factual reviewed, the calculation scheme has been repeatedly applied in peer reviewed papers /Hökmark and Claesson 2005/ and in reports that have undergone (/Hökmark and Fälth 2003/) or will undergo (/Hökmark et al. 2009/) a documented factual and quality review.

9.1.2 Freezing

Overview/general description

The overview and general description of the corresponding buffer process, Section 3.2.2, are also valid for the bentonite part of the borehole seals. In contrast to the corresponding buffer process, two new aspects must be considered:

- Freezing will occur in the borehole seals.
The extension of the frozen uppermost section of the ground during permafrost periods will vary with time and is predicted to have a maximum penetration of approximately 250 m /Hartikainen 2004/.
- A temperature gradient is imposed over the bentonite, due to the vertical geometry.
This temperature gradient, in turn, corresponds to a suction gradient and water may be transported in the bentonite to form ice lenses e.g. at the interfaces between bentonite and concrete.

When bentonite freezes, the swelling pressure will fall to zero in the temperature interval $0^\circ\text{C} < T < T_c$, where T_c is a density dependent critical temperature. For a density of $2,000$ kg/m³, the critical temperature T_c is $< -5^\circ\text{C}$. A thermal gradient below 0°C will thus correspond to a swelling pressure gradient which might cause redistribution of the bentonite.

When the pressure drop occurs, the transport paths in the surrounding rock will be frozen.

Water flow from the induced suction gradient can be estimated by identifying swelling pressure with suction:

$$\nabla \psi = -\nabla P_s = -\frac{\partial P_s}{\partial T} \nabla T \quad (9-1)$$

where ψ is suction (see Section 3.3.1). The derivative $\frac{\partial P_s}{\partial T}$ has an estimated value of 1 MPa/°C for temperatures below 0°C (see Section 3.2.2).

A typical geothermal temperature gradient is 0.025°C/m and using this value together with a value of the hydraulic conductivity of 10^{-13} m/s, the corresponding water flux is $2.5 \cdot 10^{-13}$ m/s or approximately 8 $\mu\text{m}/\text{y}$, which is also the estimated ice lens growth.

Table 9-1 summarises how the process influences and is influenced by all borehole seal variables and how these effects are treated in SR-Site.

Boundary conditions

When freezing of the bentonite in the borehole seals occurs, the water in the surrounding rock will be in ice form. Hence, transfer of water between rock and bentonite at the same level will be very limited. The slowly varying temperatures of the rock surrounding the seals also constitute a boundary condition.

Table 9-1. Direct dependencies between the process “Freezing” and the defined borehole seal variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Borehole geometry	Yes, determines the thermal boundary conditions	Included in the assessment	No	
Pore geometry	Yes	Included in the assessment	No	
Temperature	Yes	Included in the assessment	No	
Water content	Yes, via freezing point and transport capacity	Included in the assessment	Yes, If freezing takes place redistribution of water	Neglected
Gas content	(Yes)	A gas content would affect the process but the bentonite will be completely saturated when freezing	No	
Hydrovariables (pressure and flows)	Yes, freezing induces water transport	Included in the assessment	Yes	Included in the assessment
Stress state	Yes, Influences the freezing point to a small degree	Included in the assessment	Yes. Swelling pressure affected also before ice formation	Included in the assessment
Sealing materials – composition and content	Yes, via the specific surface area	Included in the assessment	No	
Porewater composition	Yes, via the specific surface area and types of counter ions	Neglected, effect assumed to be small	No	
Structural and stray materials	No		No	

Model studies/experimental studies

The general temperature response in compacted bentonite has been worked out both theoretically and experimentally in /Birgersson et al. 2010/. The same report also estimates the water transport capacity in a vertically extended bore hole seal.

Natural analogues/observations in nature

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

Time perspective

Freezing of borehole seals are relevant during the entire repository lifetime.

Handling in the safety assessment SR-Site

Because of the very restricted water transport capacity, the process is neglected.

Uncertainties

Uncertainties in mechanistic understanding

The freezing of soils is a well known process.

Model simplification uncertainties for the above handling in SR-Site

The reproducibility of the pressure response due to freezing in bentonite is good.

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

The key uncertainty is the location and duration of the permafrost front. Other uncertainties are related to the suction gradient and the assumed hydraulic conductivity. How this affects the conclusions about the process is discussed in /Birgersson et al. 2010/

9.2 Hydraulic processes

9.2.1 Water uptake and transport under unsaturated conditions

Overview/general description

Water transport in bentonite 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 bentonite. The most important driving force for water saturation under deep repository conditions is a negative capillary pressure in the pores of the bentonite 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.

For the bentonite part of the investigation holes, the process of water uptake and transport under unsaturated conditions is identical with the process described for the buffer (Section 3.3.1). There a detailed description of the process is given and it will not be repeated here.

Dependencies between process and borehole seal variables

Table 9-2 summarises how the process influences and is influenced by all variables of the bentonite seals and how these effects are treated in SR-Site.

Table 9-2. Direct dependencies between the process “Water uptake and transport under unsaturated conditions” and the defined borehole seal variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Borehole geometry	Yes	Geometry included in the models	No	
Pore geometry	Yes. Via void ratio (density) and void geometry	Variable in the model	(Yes) If erosion takes place (secondary effect)	See 9.4.10 and 9.2.4
Temperature	Yes. Indirect through water viscosity and hydrovariables in a temperature gradient	Negligible	Yes Wetting and drying affects thermal conductivity	Negligible
Water content	Yes. Via degree of saturation	Variable in the model	Yes	Variable in the model
Gas content	Yes. Via the gas pressure and degree of saturation	Variable in the model	Yes	Variable in the model
Hydrovariables (pressure and flows)	Yes. Basic variables.	Variable in the model	Yes	Variable in the model
Stress state	Yes	Variable in the model	Yes	Variable in the model
Sealing materials – composition and content	Yes. Hydraulic conductivity and retention curve etc.	Sensitivity analyses	(Yes). If erosion takes place (secondary effect)	See 9.4.10 and 9.2.4
Porewater composition	Yes	Controls some parameters in the model	Yes	Neglected, of limited importance
Structural and stray materials	(Insignificant)		No	

Boundary conditions

Interaction with the rock: The investigation holes are filled with water during emplacement and the bentonite cylinders are placed in a perforated tube during installation down into the holes. During installation the slot between the rock surface and the bentonite cylinders are filled with water with a hydraulic head equal to the hydrostatic pressure. This means that there is water enough to expand the bentonite cylinders, make them swell through the perforated holes and come in contact with the rock and only leave a small amount of unsaturated pores (~10%). The remaining water to saturate the bentonite is taken from the rock, either from fractures intersecting the hole or from the rock matrix.

Interaction with the plugs in the holes: Some parts of the holes will be grouted, stabilised and plugged with high performance, low-pH, silica concrete. The upper part will be plugged with core samples that are cast integral with the rock. These parts will not affect the wetting process.

Model studies/experimental studies

The material model that can be used for modelling the wetting phase is described in the corresponding process description for the buffer (Section 3.3.1) and will not be repeated here.

In SR-Can, no calculations of the wetting of the bentonite in the boreholes were done and are probably not needed for safety reasons, since the small size of the boreholes ensures that full saturation will be reached within five years. However, some sensitivity analyses will be done for demonstration purpose /Åkesson et al. 2010a/.

Field tests of bentonite seals in boreholes have been conducted both in Stripa and in Äspö HRL. One full scale sealing test has also been installed in Olikluoto.

Experimental studies in the laboratory of the extreme cases with no water available and excess water available should also be done in order to improve the understanding of the water uptake and homogenisation of the bentonite cylinders in the holes. Such tests have, so far, only been done with perforated copper tubes around the cylinders.

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 water will penetrate the superficial part of the bentonite cylinders that will swell and come in contact with the rock surface as a gel within a few hours. Then the water will continue to be taken up by the inner parts of the cylinders and at the same time homogenise. After less than a year, the process will be dominated by the water supply from the rock. Full saturation and homogenisation is expected to be reached within five years even in very tight rock but this should be checked with calculations.

Handling in the safety assessment SR-Site

Today's knowledge of the behaviour is judged to be sufficient for safety reasons but sensitivity analyses in combination with laboratory tests should be done in order to verify these statements.

Boundary conditions: Sensitivity analyses of the wetting with different rock properties will be done.

Handling of variables influencing this process: Most variables in Table 9-2 are included in the THM model that will be used for the modelling.

Handling of variables influenced by the process: The THM model is fully coupled so the changes in variable properties will also be considered.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

Modelling of the wetting phase is reported in a general THM modelling report that will undergo a documented factual- and quality review /Åkesson et al. 2010a/.

Uncertainties

The knowledge of the hydraulic behaviour of unsaturated bentonite material is gained from investigations done on MX-80 while almost no tests have been performed on the other candidate (Milos bentonite). At the density considered for the buffer material the behaviour should be similar.

Uncertainties in mechanistic understanding

The understanding of the process is deemed sufficient for the needs of the safety assessment. For further information; see the description of the corresponding buffer process (Section 3.3.1).

Model simplification uncertainties for the above handling in SR-Site

The same models are used and thus the same simplifications are used as for the buffer. They are less important for the seals than for the buffer (see Section 3.3.1)

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

The greatest uncertainty/variability concerns the hydraulic conditions in the near-field rock and the hydraulic interaction between the rock and the bentonite. This will be addressed by analysing a number of cases with differing assumptions regarding these properties. The data used in the modelling are discussed in the Buffer THM data report /Åkesson et al. 2010b/.

9.2.2 Water transport under saturated conditions

Overview/general description

Water transport in saturated high density bentonite 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 bentonite 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. The hydraulic conductivity K is a function of the composition of the buffer, the void ratio, e , the ion concentration in the porewater, i_c , and the temperature, T .

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

The process is identical to the corresponding process in the buffer and is further described in Section 3.3.2.

Dependencies between process and borehole seal variables

Table 9-3 summarises how the process influences and is influenced by all variables of the bentonite seals and how these effects are treated in SR-Site.

Although many variables influence the process and vice versa according to Table 9-3 the handling in the SR-Site will be that the sealed investigation holes are treated as intact rock, which means that they are disregarded in the site-scale model. The process is only important for the safety if bentonite has been lost.

Influence of density, temperature and salinity

The hydraulic conductivity is primarily dependent on the geometry and composition of the bentonite seal, the density (expressed in Table 9-3 as water content), the ion concentration in the porewater and the temperature. For further information, see Section 3.3.2.

Boundary conditions

The outer boundary conditions are determined by the hydraulic properties of the rock surrounding the investigation hole, in particular the properties of possible fractures intersecting the investigation hole.

Model studies/experimental studies

See Section 3.3.2.

Natural analogues/observations in nature

See Section 3.3.2.

Time perspective

With a hydraulic conductivity of the bentonite of 10^{-13} m/s, the borehole is at least as impermeable as the rock matrix without any fractures. This means that even with an impossible axial hydraulic gradient of 1, the time for water to flow from the repository level along the borehole up to the surface would take in the order of 100 million years. Freezing is treated separately.

Table 9-3. Direct dependencies between the process “Water transport under saturated conditions” and the defined borehole seal variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Borehole geometry	Yes, mainly by the flow path.	Given as input data.	Yes, during swelling since water flow into the voids makes the bentonite swell if there is space available.	Included in the mechanical model
Pore geometry	Yes, determines the hydraulic conductivity	Included in the value of the hydraulic conductivity as a function of the density. The pore geometry can be affected by a mineral transformation or a change in porewater composition.	Yes, during swelling since water flow into the voids makes the bentonite swell if there is space available.	Included in the mechanical model
Temperature	Yes, through water viscosity and at temperature below 0 (see Freezing).	This will be neglected in SR-Site	Insignificantly.	No
Water content	Influenced via density (pore geometry)	Determines the hydraulic conductivity, which is included in the model.	Yes, during swelling since water flow into the voids makes the bentonite swell if there is space available.	Included in the mechanical model
Gas content	Insignificantly (dissolved gases)	Excluded since it would reduce hydraulic conductivity	No	
Hydrovariables (pressure and flows)	Yes, main variables.	Included in the flow model	Yes	Included in the flow model
Stress state	Yes. If the effective stress on the bentonite deviates from the swelling pressure the bentonite will change volume and water will flow into or out from it.	Included in the mechanical model.	Yes	Included in the mechanical model
Sealing materials – composition and content	Yes, determines the hydraulic conductivity	Included in the model	No	
Porewater composition	Yes, determines the hydraulic conductivity	Included in the model	Yes	Replacement of porewater is discussed in 3.5.6
Structural and stray materials	(Insignificant)		No	

Handling in the safety assessment SR-Site

As illustrated by the time perspective the water flow along the holes can be neglected as long as the bentonite remains its low hydraulic conductivity. This case will thus not be further handled in SR-Site. If there is a risk that a large part of the bentonite will be lost or transformed to obtain other properties, these cases must be handled. Cases with unsealed boreholes are discussed in the Geosphere Process Report /SKB 2010i/.

The primary handling of these cases will be to consider how the hydraulic conductivity could vary for the evolving conditions in the bentonite seal throughout the assessment period.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

No references are used.

Uncertainties

So far, very few tests have been performed on Deponit CA-N bentonite, but the 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 also Section 3.3.2.

9.2.3 Gas transport/dissolution

Overview/General description

Gas processes in the borehole seals are only relevant for the saturation period and only for the bentonite part of the seal – this is described in Section 3.3.3.

Handling in the safety assessment SR-Site

The process is included in the supporting sensitivity analyses of the saturation phase see Section 9.2.1.

9.2.4 Piping/erosion

Overview/general description

As described for the corresponding buffer process (Section 3.3.4), piping and erosion are primarily a problem in the unsaturated stage when water flows between different parts of rock cavities. Since the investigation holes are filled with water from start, erosion will not take place after installation. There are no high axial hydraulic gradients along the hole so there will be no axial water flow that can erode the bentonite. Any large fracture zones that may cause flow along the investigation hole during installation are presupposed to be grouted and sealed.

Handling in the safety assessment SR-Site

Since piping and erosion of the bentonite cannot occur in stagnant water, the process is ruled out for the seals in the investigation holes.

However, there is a risk for abrasion of the material during the installation phase. This is discussed in the Closure production report /SKB 2010f/

The long term erosion by colloid transport is treated in Section 9.4.10

9.3 Mechanical processes

9.3.1 Swelling/mass redistribution

The swelling process has been merged with other stress-strain-related processes that can cause mass redistribution within the borehole seals namely thermal expansion, creep and a number of interactions.

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.

The process of swelling and mass redistribution is described in detail with all influences and dependencies in the buffer Chapter (Section 3.4.1) and will not be repeated here. Instead, a brief description of the mechanical evolution of the bentonite cylinders in the investigation holes is provided.

During placement of the bentonite cylinders confined in the perforated copper tube into the hole, the slot between the cylinder and the rock surface is filled with water with a water pressure with a magnitude that depends on the depth (0-10 MPa water pressure). The high water pressure in combination with the high suction in the bentonite means that the surface of the cylinders will be wetted immediately and there will be a gel expanding from the surface. After less than a few hours, the gel will come in contact with the rock wall but the water will continue to penetrate into the cylinder and make more bentonite swell. In this way the gel will consolidate and increase its density at the same time as the bentonite cylinder slowly decreases its density, at first locally close to the surface and then deeper and deeper.

Due to the perforated copper tube around the bentonite cylinders the swelling will be rather inhomogeneous. The swelling will at first go through the holes and out to the rock surface and then along the rock wall between the tube and the rock wall and fill up the remaining parts. The influence of the copper tube on the wetting rate is insignificant compared to if there were no tube but the density distribution at end state will differ significantly due to the friction in the bentonite that will prevent homogenisation. The density between the tube and the rock wall will be much lower than the average density but still high enough to function as a seal.

There are a combined saturation, swelling and homogenisation of the bentonite that takes place even if there is no additional water available for the bentonite. This process is complicated and difficult to model. Some tools (Code Bright and Abaqus) are available and further developments are ongoing. The process that may take up to a few years, depending on the availability of water, ends when the bentonite is saturated and the radial pore pressure distribution equalised. The swelling pressure against the rock will increase with time and is estimated to end at between 2 and 5 MPa.

Dependencies between process and borehole seal variables

Table 9-4 summarises how the process influences and is influenced by all variables of the bentonite seals and how these effects are treated in SR-Site.

Table 9-4. Direct dependencies between the process “Swelling/mass redistribution” and the defined borehole seal variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence (How/Why not)	Influence present? (Yes/No) Description	Handling of influence (How/Why not)
Borehole geometry	Yes	Geometry included in the models	No	
Pore geometry	Yes. Through stress state and void ratio	Included in the models	Yes	Included in the models
Temperature	Yes. Thermal expansion and change of retention properties (especially at temperatures below 0).	No, negligible	No	
Water content	Yes.	Variable in the model	Yes	Variable in the model
Gas content	Yes. Degree of saturation and gas pressure	Included in the models	Yes	Included in the models
Hydrovariables (pressure and flows)	Yes. Basic variables.	Variable in the model	Yes	Variable in the model
Stress state	Yes	Variable in the model	Yes	Variable in the model
Sealing materials – composition and content	Yes. Determines many parameters in the models	Sensitivity analyses	No	
Porewater composition	Yes. Influences many parameters in the models	Sensitivity analyses	No	
Structural and stray materials	No		No	

As shown in Table 9-4, there are many variables that affect the mechanical behaviour and which are included in the mechanical models. These dependencies are described for the corresponding buffer process (Section 3.4.1) and will not be repeated here.

Boundary conditions

The mechanical boundary conditions and interactions are limited since the borehole implies a very stiff confinement with no complications.

Interaction with the rock

The following mechanical interactions between the bentonite in the investigation holes and the rock have been identified:

- 1. Swelling pressure from the buffer** is transferred to the rock but is not expected to lead to any rock movements. The elastic deformation of the rock at the expected swelling pressures is small due to the rock's high modulus of elasticity (about 70 GPa).
- 2. Forces of friction** between the bentonite and the rock surface will occur along the borehole in the unperforated parts of the copper tube. Axial friction can also occur if there are concrete seals that are partly dissolved.
- 3. Thermal expansion of the buffer** may cause stresses on the rock if the bentonite is water-saturated when the temperature increase occurs. The slow temperature increase in combination with the drainage through the rock implies that this effect is insignificant.
- 4. Convergence of the holes** will occur with time but the effect is insignificant.
- 5. 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. This interaction is treated in Section 3.4.1. It may also occur due to the colloid transport out from the fracture (see Section 9.4.10). Since the mass of bentonite in the hole at the intersecting fractures is small this may entail local problems with complete loss of bentonite at the fracture. However, the problem is judged to be local since the friction between the rock and the bentonite will prevent mass transfer axially. A sensitivity calculation of these effects should be done.

Interaction with concrete plugs and concrete stabilised parts of the hole.

If the concrete degrades and cement is transported away there may be extra space for swelling bentonite. However, this is judged to be a minor problem since the effect is local. Some sensitivity calculations should be done.

Model studies/experimental studies

A large number of experimental studies and model studies of the mechanical properties of both unsaturated and saturated bentonite have been performed. These are treated in the buffer process Section (3.4.1).

Regarding the behaviour of plugged boreholes, field tests of bentonite seals in boreholes have been made both in Stripa and in Äspö HRL. One full scale sealing test has also been installed in Olikluoto.

Time perspective

The water saturation phase is expected to take less than a few years, depending on the properties of the rock. During this time span, the portion of the expansion and homogenisation that is limited by the consolidation rate (which is controlled by the hydraulic conductivity) also takes place.

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-Site

Mainly three studies should be done for SR-Site:

1. Analytical modelling of the homogenisation process related to the swelling of bentonite through the perforated copper tube
2. Modelling and sensitivity analyses of the saturation processes from installation until equilibrium is reached.
3. Modelling and sensitivity analyses of the effect of local loss of bentonite.

The effect of an un-sealed borehole will be illustrated in SR-Site.

Adequacy of references supporting the suggested handling in the safety assessment SR-Site

Modelling of the three cases is reported in a general THM modelling report that will undergo a documented factual- and quality review /Åkesson et al. 2010a/.

Uncertainties

Uncertainties in mechanistic understanding

See the buffer process 3.4.1

Regarding the homogenisation process there are uncertainties in the analytical models and the friction coefficient but comparisons with measurements have to some extent confirmed the models.

Model simplification uncertainties for the above handling in SR-Can

See the buffer process 3.4.1 and uncertainties in mechanistic understanding.

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

See the buffer process 3.4.1 and uncertainties in mechanistic understanding.

9.3.2 Liquefaction

Overview/general description

Liquefaction in the buffer is described in Section 3.4.2 and is not further addressed here.

Handling in the safety assessment SR-Site

The process is ruled out for the bentonite in the investigation holes and would if it could occur not have any influence on the performance.

9.4 Chemical processes

9.4.1 Advective transport of species

In this context, advection refers to transport of any forms of additional matter, e.g. ions, molecules or colloids, with porewater flow. The transport direction is thereby principally from volumes of high water pressure to volumes of lower pressure. The process leads to redistribution of solutes in the porewater and thus affects the porewater composition. There are several possible causes of pressure gradients in the borehole seals, e.g. external water pressure, affinity for water in the bentonite and temperature induced volume change of the water. Advection is closely related to water flow in the borehole seals, which is described in Section 9.2.2. Advection may though be different compared to pure water flow due to ion equilibrium effects in the case of ions, and due to filtering by nano-sized pores in the case of colloids.

Advective transport is of importance in the bentonite part of the borehole seals during the saturation period. Under saturated conditions, the transport of solutes in the bentonite porewater is expected to be dominated by diffusion, see Section 9.4.2. Advective flow will probably be significant in the cement/sand parts of the seals in the long term perspective due to cement degradation.

Dependencies between process and borehole seal variables

Table 9-5 summarises how the process influences and is influenced by all borehole seal variables and how these effects are treated in SR-Site.

Boundary conditions

The external boundary condition for this process is the hydraulic gradient and the concentration gradients for species across borehole seals. In principle, the difference between two fractures intersected by a plug is of main interest, since the difference within one fracture will be insignificant on the length scale of the borehole seal.

Model studies/experimental studies

Field studies of borehole seals are ongoing by SKB and Posiva in Äspö and Olkiluoto.

Table 9-5. Direct dependencies between the process “Advective transport of solutes” and the defined borehole seal variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable			
	Influence present? (Yes/No)	Description	Handling of influence (How/Why not)	Influence present? (Yes/No)	Description	Handling of influence (How/Why not)
Borehole geometry		The geometry of the boreholes determines the cross-section available for advection.	Included in model	Yes, through dissolution/precipitation		Of no concern
Pore geometry	Yes, dominating effect	through hydraulic conductivity in both bentonite and concrete		Yes, through dissolution/precipitation		Included in model
Temperature	Insignificant			Insignificant		
Water content	Yes, by definition		Assumed to be saturated	Insignificant		
Gas content	Yes, by reduction of transport paths, through dissolution/precipitation of gas		Assumed to be saturated	Yes, dissolution/release of gas		Assumed to be saturated
Hydrovariables (pressure and flows)	Yes, by definition		Included in model	Yes, through osmosis		Advection only considered after loss of bentonite
Stress state	Indirectly through pore geometry			Yes, through osmosis in the bentonite		Advection only considered after loss of bentonite
Sealing materials – composition and content	The content of montmorillonite is of decisive importance in the bentonite part. Indirectly through dissolution/precipitation process in the concrete part		Advection only considered after loss of bentonite	Yes, through precipitation/dissolution and ion exchange processes		Of no concern
Porewater composition	Yes, by definition		Advection only considered after loss of bentonite	Yes, by definitions		Only radionuclide transport considered
Structural and stray materials	(Insignificant)			No		

Natural analogues/observations in nature

No relevant studies available.

Time perspective

Advective flow transport is important on all timescales. Significant flow will take place in the cement/sand parts after degradation of the cement.

Handling in the safety assessment SR-Site

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 will be considered when defining initial conditions for modelling of the chemical evolution after saturation.

Open boreholes will be considered as a variant in the hydrogeological modelling.

Handling of variables influencing this process:

See section 9.2.2

Uncertainties

Uncertainties in mechanistic understanding

See Section 9.2.2 for uncertainties concerning water advective transport.

Model simplification uncertainties SR-Site

Saturated conditions: The process can be modelled with a standard mass-transfer approach.

Input data and data uncertainties in SR-Site

See Section 9.2.2

9.4.2 Diffusive transport of species

An overview of diffusion processes and phenomena as relevant for bentonite and concrete are given in Sections 3.5.3 and 8.4.2, respectively, these considerations also apply to the concrete- and bentonite-parts of the borehole seals. /Luna et al. 2006/ conclude that the main diffusion parameters (incl. porosity) will not be significantly affected by an alkaline plume.

Dependencies between process and borehole seal variables

Table 9-6 shows how the process influences and is influenced by all system variables.

Influence on variables of borehole seals: Through transport of dissolved species to and from the concrete/bentonite system, diffusion will influence the overall composition and rate of alteration.

Influence of variables of borehole seals: Analogous to buffer in case of bentonite; analogous to the concrete part of bottom plates in case of the concrete part (Sections 3.5.3 and 9.4.2; respectively).

Boundary conditions

A possible transfer of species from the repository system to a borehole seal can be visualised as the diffusion of dissolved species from one porous medium to another. The transfer of species from the seal to the geosphere can be visualised as the diffusion of dissolved species from the clay or concrete into flowing water (equivalent flow rate or Q_{eq}).

Table 9-6. Direct dependencies between the process “Diffusive transport of species” and the defined borehole seal variables and a short note on the handling in SR-Site.

Variable	Variable influence on process		Process influence on variable	
	Influence present? (Yes/No) Description	Handling of influence? (How/why not)	Influence present? (Yes/No) Description	Handling of influence? (How/why not)
Borehole geometry	Yes	Diffusion is neglected in bore hole seals	No	
Pore geometry	Yes, Reflected in the magnitude of diffusion coefficients	Diffusion is neglected in bore hole seals	Possibly indirectly through influence on porewater composition	
Temperature	Yes, influence of temperature on diffusion in must be acknowledged, but is not included (effect is not established for concrete and considered as small for bentonite)	Diffusion is neglected in bore hole seals	No	
Water content	Yes	Diffusion is neglected in bore hole seals	No	
Gas content	Saturated conditions assumed		For dissolved gases such as CO ₂ , CH ₄	Neglected
Hydrovariables (pressure and flows)	Saturated conditions assumed		No	
Stress state	Indirectly through pore geometry		Possibly indirectly through influence on porewater composition/ mineral equilibria/ swelling	Neglected
Bentonite and concrete composition	Yes, defines magnitude of diffusivities	Diffusion is neglected in bore hole seals	Possibly indirectly through influence on porewater composition/ mineral equilibria	Neglected
Porewater composition	Through effect on speciation and extent of EDL in bentonite, Defines magnitude of diffusivities	Diffusion is neglected in bore hole seals	Through diffusive transport of main dissolved constituents	Neglected

Model studies/experimental studies

Diffusion in the bentonite part of the borehole seals is analogous to diffusion in the buffer and diffusion in the concrete parts of the seals is analogous to diffusion in the concrete part of bottom plates (Sections 3.5.3 and 8.4.2, respectively).

Time perspective

Diffusion could be active in all time perspectives.

Natural analogues/observations in nature

Diffusion in the bentonite part is analogous to diffusion in the buffer, see Section 3.5.3.

Handling in the safety assessment SR-Site, uncertainties

Transport of species with diffusion in the borehole seals is not considered.

Uncertainties

Not applicable.

9.4.3 Sorption (including exchange of major ions)

Overview/general description

Seals of investigation boreholes consist of bentonite in copper tubes, plus low-pH concrete in the conductive areas. The sorption processes taking place in these systems are the same as in other bentonite and concrete parts of the repository system and are described in Sections 3.5.5 and 5.4.3 and 8.4.3, respectively. The effects of concrete-bentonite interaction and the behaviour of organic concrete admixtures are described in Section 5.4.3.

Handling in the safety assessment SR-Site

Sorption of radionuclides is neglected both in the concrete and the bentonite parts of the borehole seals. No radionuclide transport is assumed to take place in an intact seal. In the case of a defect seal, sorption is conservatively neglected.

9.4.4 Alteration of concrete

Overview/general description

This process is in general identical with the corresponding alteration process for concrete in the tunnel plug (Section 5.4.4).

Handling in the safety assessment SR-Site

The pH evolution from the concrete part of the borehole seals will in most respects be identical to the effect from the plugs (Section 5.4.4). Therefore, the results from modelling of the pH evolution in and around the concrete plugs will be used to draw conclusions regarding the pH evolution in and around borehole seals. The evolution of the hydraulic properties of the seals will be studied in a sensitivity analysis, see Section 9.2.2.

9.4.5 Aqueous speciation and reactions

Overview/general description

This process is in general identical with the corresponding process in the buffer (Section 3.5.7).

Handling in the safety assessment SR-Site

The process is included in a separate modelling task of the seal (concrete part) degradation, which in principle is the same as the plug degradation. This is further described in Section 5.4.4.

9.4.6 Copper corrosion

Overview/general description

Corrosion of copper is described in the Fuel and Canister Process Report /SKB 2010k/ (process copper corrosion).

Handling in the safety assessment SR-Site

The copper pipes are only important during installation of the borehole seals. No assessment of the copper in the seals will be done in SR-Site.

9.4.7 Alteration of impurities in bentonite

Overview/general description

The bentonite material consists not only of montmorillonite, but also of accessory minerals as well as impurities. In the system under consideration, these can be dissolved and sometimes re-precipitated depending on the prevailing conditions.

The reactions relevant for the borehole seals are basically the same as those in the buffer (Section 3.5.6). However, there are a few differences in the significance of the processes.

- The temperature is lower and the thermal gradient in the borehole seal is small. Dissolution/precipitation of minerals due to temperature effects are of minor importance in the seals.
- The total volume of bentonite in a seal is much less than in a deposition hole. Therefore the effects of changes in groundwater chemistry will be much faster.
- The borehole seals are not in direct contact with the deposition holes and changes in the porewater chemistry will not affect the barriers in the repository

The geochemical evolution of the bentonite part of the borehole seal will be equivalent to that of the bentonite buffer (see Section 3.5.6 on alteration of impurities of the buffer system part), and therefore it can be used as analogue.

Handling in the safety assessment SR-Site

As described above, the geochemical evolution in the borehole seals will be of limited importance for the performance of the repository. The process is therefore neglected in SR-Site. (The results from the modelling geochemical evolution in the buffer can be used as an analogue).

9.4.8 Osmosis

Overview/general description

See buffer Section 3.5.8

Osmosis is of importance only in the bentonite component of the borehole seals.

Handling in the safety assessment SR-Site

The salinity of the groundwater will affect the swelling pressure of the bentonite parts of the seals. This will be evaluated in the main report of SR-Site in a similar manner to the same process for the buffer, see buffer Section 3.5.8

9.4.9 Montmorillonite transformation

Overview/general description

Temperature, which is a main factor in montmorillonite transformation in nature, will be relatively low in the montmorillonite parts of the seals and no significant hydrothermal alteration is consequently expected. Possible threats are high pH solutions from cement, which may lead to dissolution of the montmorillonite, see buffer Section 3.5.9. However, the cement is supposed to be of low pH type.

Handling in the safety assessment SR-Site

The stability of the montmorillonite itself and the interaction between low-pH cement and bentonite is handled in the same way as for the buffer, see Section 3.5.9.

9.4.10 Montmorillonite colloid release

Overview/general description

The process is the same as for the buffer (Section 3.5.11).

Handling in the safety assessment SR-Site

In the case of diluted waters, loss of bentonite from the borehole seal cannot be excluded. Open boreholes will be treated as a case in the hydrogeological modelling. See also Section 9.2.2.

9.4.11 Microbial processes

Overview/general description

It is not foreseen that microbial processes can interfere with the seals in a way that will influence the performance of the repository.

Handling in the safety assessment SR-Site

Microbial processes in the borehole seal is not treated in SR-Site. Sulphate reducing bacteria could potentially affect the copper tubes, but since these have no intended performance after installation, the process can be neglected.

9.5 Radionuclide transport processes

9.5.1 Speciation of radionuclides

Overview/general description

See corresponding process description for the buffer, Section 3.6.1

Handling in the safety assessment SR-Site

This process is indirectly handled through the selection of parameters for radionuclide transport in the rock. In general, the handling of the process is the same as for the corresponding process in the geosphere, see process Transport of radionuclides in the water phase in the Geosphere Process Report /SKB 2010i/.

9.5.2 Transport of radionuclides in the water phase

Overview/general description

If the borehole seals work as intended they do not have to be considered in the radionuclide transport calculations. If not, they are represented as a pipe with high hydraulic conductivity in the geosphere transport model.

Handling in the safety assessment SR-Site

The borehole seals are considered to be a part of the rock in the radionuclide transport calculations. See process Transport of radionuclides in the water phase in the Geosphere Process Report /SKB 2010i/.

10 References

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