SKI Report 2005:48

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Engineered Barrier System - Long-term Stability of Buffer and Backfill

Report from a Workshop in Lund, Sweden, November 15-17, 2004

Synthesis and extended abstracts

Swedish Nuclear Power Inspectorate
September 2005

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Foreword

SKI is preparing to review the license applications being developed by the Swedish Nuclear Fuel and Waste Management Company (SKB) for an encapsulation plant and a deep repository for the geological disposal of spent nuclear fuel (SFL-2). As part of its preparation, SKI is conducting a series of technical workshops on key aspects of the Engineered Barrier System (EBS) of the repository. This workshop concerns the long-term stability of the buffer and the backfill. Previous workshops have addressed the overall concept for long-term integrity of the EBS (SKI report 2003:29), the manufacturing, testing and QA of the EBS (SKI report 2004:26) and the performance confirmation for the EBS (SKI report 2004:49). The goal of this work is to achieve a comprehensive overview of all aspects of SKB's EBS work prior to the handling of forthcoming license applications. The reports from the EBS workshops will be used as one important basis in future review work.

The workshops involve the gathering of a sufficient number of independent experts in different subjects of relevance to the particular aspect of EBS. A workshop starts with presentations and discussions among these experts. Following this, SKB presents recent results and responds to questions as part of an informal hearing. Finally, the independent experts and the SKI staff examine the SKB responses from different viewpoints. This report aims to summarise the issues discussed at the buffer and backfill workshop and to extract the essential viewpoints that have been expressed. The report is not a comprehensive record of the discussions and individual statements made by workshop participants should be regarded as opinions rather than proven facts.

This reports includes apart from the workshop synthesis, questions to SKB identified prior or during the workshop, and extended abstracts for introductory presentations. The main part of the work with the synthesis has been done by Mick Apted (Monitor Scientific LLC), Randy Arthur (Monitor Scientific LLC) and Dave Savage (Quintessa).

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1. Introduction

SKI is preparing to review the license applications being developed by the Swedish Nuclear Fuel and Waste Management Co. (SKB) for an encapsulation plant and a deep repository for the geological disposal of spent nuclear fuel (SFL-2). As part of its preparation, SKI is conducting a series of technical workshops on key aspects of the Engineered Barrier System (EBS) of the repository. Multiple objectives for these workshops include:

- identifying technical issues that are likely to be particularly important in future reviews,
- listing key technical analyses and supporting information that SKB should include in their license applications,
- identifying the time schedule over which different issues need to be addressed by SKB,
- guiding future research efforts, such as model development, and performance confirmation experiments to support the licensing process in a timely and effective manner.

Furthermore, SKI uses these technical workshops to integrate the multiple scientific and engineering disciplines needed to satisfactorily evaluate the long-term contribution to safe waste isolation of the different engineered barriers of the EBS.

In November 2004, a workshop was conducted in Lund, Sweden, focusing on the long-term stability of buffer and backfill components of SKB's proposed EBS. These barriers are shown in Figure 1 for the proposed KBS-3 type of repository. Detailed descriptions of the buffer and backfill, as well as their intended functions within the EBS, are presented by SKB in their "SR-CAN Interim Process Model" report (SKB, 2004).

The buffer will consist of blocks of compacted bentonite (i.e., a natural material composed dominantly of a swelling smectite clay called montmorillonite) to protect copper-based spent fuel canisters. The swelling character of montmorillonite arises from the entry of water along layers in the clay structure. The hydraulic properties of the buffer should preclude groundwater flow and the mechanical properties should be such that any (minor) movement in the bedrock would not harm the canister. A secondary function of the buffer is to limit radionuclide transport if the isolation of a canister would for some reason be broken. However, this workshop focussed only on the primary buffer function to protect the canisters.

The backfill is currently expected to be composed of an aggregate of bentonite and crushed rock, but other similar materials are also considered (such as Friedland clay). The intended function is restricting possible groundwater flow through the deposition tunnels located above the canister deposition holes. Rapid groundwater flow in the tunnels would be unfavourable from a radionuclide transport point of view. The backfill is also needed to restrict the upward expansion of the swelling buffer material, to avoid a harmful reduction of the buffer density. The requirements and functions will be less demanding for the backfilling of other tunnels such as ramps, shafts and access tunnels. This workshop did not address these issues, apart from concluding that more information will be needed about this topic as well.

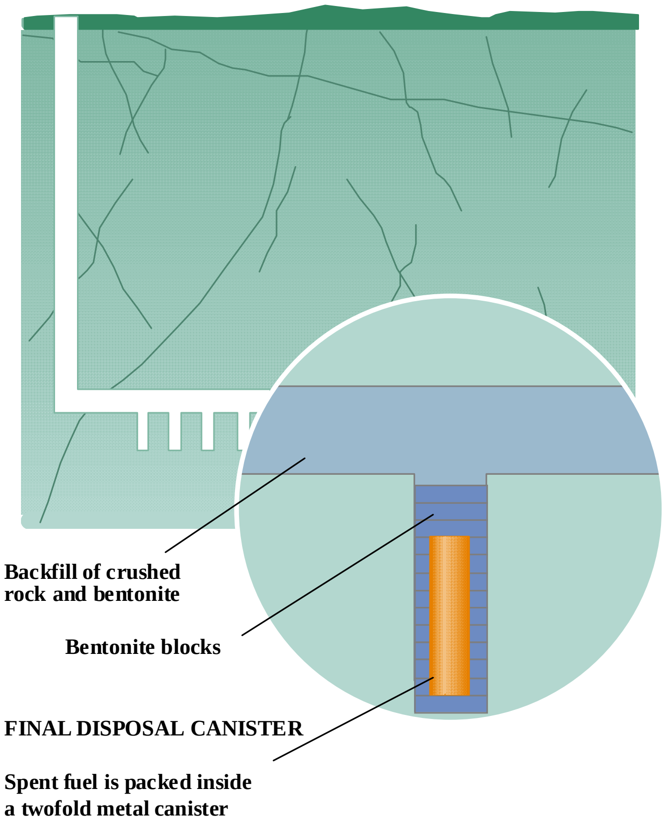

Figure 1. Schematic cross section of a KBS-3 type repository showing placement of buffer and backfill material within deposition holes for spent-fuel canisters.

2. Workshop format

The overall agenda and participants for the buffer and backfill workshop, with professional affiliation and technical expertise, are provided in Appendix A. As part of its planning, SKI first solicited review questions to be posed to SKB from its technical staff and support contractors. These seven extended questions are provided in Appendix B of this report. In addition to these questions SKI provided a list of “be aware questions”. These were issues for SKB to be prepared to discuss, as it was considered likely that they would be raised at the meeting. No formal presentations were required by SKB in advance. SKI’s objectives for preparing and submitting these comments to SKB prior to the workshop were:

- to identify critical questions and possible gaps in SKB’s information about the EBS,
- to allow SKB reasonable time prior to the workshop to prepare full responses to questions,
- to summarise outstanding issues that may require further consideration and analysis by SKI, based on SKB responses,
- to ensure that SKB could at an early stage identify suitable staff and technical experts for participation in the informal hearing of the workshop.

On the first day of the buffer and backfill workshop, SKI and its contractors met to discuss key issues that had already been identified in previous discussions. SKI staff reviewed the current regulatory schedule in Sweden for the encapsulation plant and the repository for spent nuclear fuel. Short presentations dealing with potential buffer and backfill issues were also made and discussed by SKI’s consultants. These topics corresponded mainly to ongoing and completed research projects financed by SKI. Extended abstracts for the presentations are provided in Appendix C.

In the afternoon, SKI and its consultants divided into two working groups, one for the buffer and one for the backfill. Each group reviewed the prepared questions in order to clarify their intent, and to prepare follow-up questions in anticipation of SKB’s formal responses. Clay Technology AB, a company providing key technical support to SKB’s R&D program on buffer and backfill issues, hosted an evening session in which orientation talks were given on experimental techniques and current research projects. This was followed by an open tour of their laboratory and test facilities. A large-scale test for the horizontal option of buffer and canister emplacement (KBS-3H) was also shown (the “Big Bertha” experiment).

During the second day of the workshop, SKB and its technical contractors made formal presentations on all of the SKI questions in a morning session. These presentations are summarized in subsequent sections. Each presentation was followed by a question period for clarification of minor issues. In the afternoon session, SKI and its consultants carried out an informal hearing with SKB staff and its contractors, based on the detailed questions developed on the first day of the Workshop (Appendix B). The subsequent sections include brief summaries of the discussions associated with the various topics. The intent has not been to write down a comprehensive record of these discussions, but rather to single out issues and topics that may be important in the upcoming licensing reviews. In the evening, Professor Roland Pusch gave a lecture to the SKI and its consultants, entitled “Long-term characteristics of the clay barrier, assumptions and knowledge”. In particular, this talk provided background and context for the issues of bentonite illitisation and cementation.

For the third and final day of the workshop, SKI and its consultants met to discuss SKB’s responses to questions posed at the workshop, to debate the current status of identified issues, and to identify and prioritize remaining concerns regarding buffer and backfill issues. These discussions and recommendations are presented in the concluding section of this report. Finally, the workshop included an optional visit to the factory for fabrication of bentonite blocks in Ystad.

3. Function indicators

3.1 General aspects

A function indicator is a concept recently developed and implemented to simplify the evaluation of long-term performance for a spent fuel repository (e.g. SKB, 2004). Although dose and risk compliance criteria are the ultimate measures of safety and regulatory compliance, SKB will also as a repository implementer benefit from evaluation of their planned repository system and associated safety concept in a more detailed and disaggregate manner. Such evaluation of certain functions, considered separately and independently of a full safety assessment, that are thought to be important determinants of safety may also facilitate the review of SKB's safety case. SKB believe that the use of function indicators can help to focus research and development efforts and should simplify the safety assessment since certain processes can be excluded if selected criteria are fulfilled.

The SKB approach is to identify and define a number of function indicators, especially for the near-field components in their repository concept. Measurable properties of components, or those that can be calculated, have also been defined as criteria for each function indicator. SKB believes that if the criteria are met a ”good” or satisfactory performance of that particular component will be assured.

SKB noted that it expects that the criteria and function indicator will be met throughout the assessment period, unless otherwise explicitly restricted to a specific time period. Specific examples were made of buffer/backfill function indicators during the early period of re-saturation and elevated temperature in the repository, compared to function indicators for the longer-term period when the impacts of glacial cycles on repository performance must also be evaluated.

Fulfilment of function-indicator criteria alone, notes SKB, will not guarantee repository safety because repository and barrier performance cannot be readily captured by a simple comparison to a criterion. A system-level analyses of the integrated multiple barriers is needed for that. Conversely, the repository may be safe despite violation of one or several criteria, because of the balancing effect of additional engineered and natural barriers. In cases where a function indicator was not met, however, SKB indicated a more elaborate analysis would be conducted. SKB also noted that certain aspects of repository evolution could not be captured with simple criteria, and that other methods apart from function indicators would have to be used in such cases.

Workshop participants felt that function indicators could be an important new concept for focussing the coming safety assessment work. Their role in a safety assessment context is not entirely clear, however. It is conceivable, for example, that future assessments could demonstrate safety with respect to the dose/risk compliance criterion even if certain function-indicator criteria are not met. This apparent disconnection from safety assessment results could appear to be confusing and the concept of “a criterion” could perhaps convey an incorrect meaning. Moreover, the different characteristics of various function indicators were noted, such as temperature (an intensive state variable) and hydraulic conductivity (a materials property). This makes it more difficult to assess the combination of suggested function indicators. It is therefore essential for SKB to clearly explain and justify the selection of function indicators, and to exclude the possibility of a more suitable and well-defined alternative set of function indicators. The completeness of SKB's set of function indicators must also be evaluated once its exact purpose in a safety assessment context is clarified.

SKB was also asked about the derivation of specific criteria values, and acceptable margins for uncertainties in these values. SKB replied that this information will be available in the so called "Process Report", which will be one of the main references supporting the upcoming SR-Can and SR-Site safety assessments. In addition to past sensitivity analyses on key properties, SKB also stated its plans to continue to conduct such sensitivity analyses to demonstrate that safety will be assured for the ensemble set of stated criteria values. SKB noted its willingness to expand the current list of function indicators, but that a key requirement in any such action would be to demonstrate a strong connection to repository performance and safety.

Workshop participants asked about the time dependency and coupling of function indicators. According to SKB, time dependency is built into the concept because the indicators have to be fulfilled during the entire assessment period of 1 million years. SKB stated that they have considered coupled effects on function indicators insofar as such effects are known and can be quantified. No mutually exclusive function indicators have yet been discovered, but careful consideration is needed to avoid conflicts in their quantitative specification (e.g., selecting repository depths that are deep enough to avoid freezing of buffer/backfill, but shallow enough to minimize high, or anisotropic, in-situ rock stresses).

3.2 Bentonite buffer

Table 1 lists SKB's preliminary set of function indicators for the buffer. Table 2 shows a set of complementary indicators for the surrounding rock, which have direct implications for the function of the buffer. SKB described the rationale for the buffer function indicators and the basis (experimental and modelling results) for the selected criteria. Aspects such as diffusive transport (hydraulic conductivity, swelling pressure), temperature, mechanical indicators (canister sinking, protection against shear), microbial activity, and colloid transport were discussed. Several of these are related to the dry density of the emplaced bentonite blocks, which is therefore a parameter that must be optimised. SKB have not yet been able to define function indicators for gas transport and the radionuclide transport attenuation. It is not yet clear whether these indicators are needed.

Workshop participants noted that a buffer density criterion for the avoidance of canister sinking was missing from Table 1. SKB explained that it is hard to derive a quantitative criterion for this purpose based on modelling results, and considered the likelihood of such an event to be very small. This will be addressed in the upcoming SR-Can reports. Alternatives for some of the function indicators were discussed. For example, specification of a maximum thermal gradient might be more relevant to the long-term performance of the buffer than specification of a maximum absolute temperature. SKB acknowledged that the gradient may be important, but suggested that it is not possible to define a definite criterion.

It was suggested that suspected or confirmed non-compliance with a given function indicator should be documented, not only because additional evaluation and modelling work would be needed but also because design changes might be needed. Consideration of various design options could be partially based on evaluation of function indicators.

Table 1. SR-CAN table of Function Indicators, with associated Criteria, for buffer.

Function indicator	**Criterion**	**Rationale**
Buffer		
Bulk hydraulic conductivity	$k^{Buff} < 10^{-12}$ m/s	Avoid advective transport in buffer
Swelling pressure	$k_{Swell}^{Buff} > 1$ MPa	Ensure tightness, self healing
Maximum temperature	$T^{Buffer} < 100°C$	Ensure buffer stability
Minimum temperature	$T^{Buffer} > 0°C$	Avoid freezing
Buffer density around entire canister	$\rho_{Bulk}^{Buff} > \rho_{Sink}$ kg/m^3	Avoid canister sinking (criterion to be determined)
Buffer density around entire canister	$\rho_{Bulk}^{Buff} > 1800$ kg/m^3	Exclude microbial activity
Buffer density around entire canister	$\rho_{Bulk}^{Buff} > 1650$ kg/m^3	Prevent colloid transport through buffer
Buffer density around entire canister	$\rho_{Bulk}^{Buff} < 2100$ kg/m^3	Ensure protection of canister against rock shear

Table 2. SR-CAN table of Function Indicators, with associated Criteria, for rock.

Function indicator	**Criterion**	**Rationale**
Rock		
Minimum ionic strength	$\sum [M^{2+}]^{GW} > 10^{-3}$ M (Total divalent cation conc.)	Avoid buffer erosion
Limited alkalinity	$pH^{GW} < 11$	Avoid dissolution of buffer smectite
Limited salinity	Buffer: [NACl]< 100 g/l Backfill: [NaCl]< 35 g/l (Or other compositions of equivalent ionic strength)	Avoid detrimental affects, in particular on buffer and backfill swelling pressures
Limited concentration of detrimental agents for buffer and canister	Applies to HS^-, K^+ and Fe. The lower the better (no quantitative requirement)	Avoid canister sulphide corrosion, avoid illitisation (K^+) and chloritisation (Fe) of buffer and backfill

3.3 Backfill

Table 3 lists function indicators for the backfill. The complementary function indicators for the rock, presented in table 2 are also of relevance in the backfill context. The only difference is that the backfill is associated with a more strict requirement for maximum salinity (which should therefore be the limiting case). There are significantly fewer function indicators for the backfill than for the buffer, reflecting its less pronounced role in assuring long-term containment. Examples of this role include keeping the buffer in its place (providing sufficient buffer density) and avoiding preferential flow along deposition tunnels. This can be compared with the primary role of the buffer to protect the copper canister and to limit the subsequent diffusive-release rate of radionuclides.

Workshop participants asked whether an extended storage of crushed rock at the surface would affect the properties of these materials for use as backfill components. SKB acknowledged that this must be studied, but no results are available yet.

Workshop participants were concerned that there might be a contradiction between the compressibility and hydraulic conductivity requirements for the backfill. According to a previous SKB report, decreasing the fraction of crushed rock in order to decrease hydraulic conductivity (by increasing the clay fraction) would increase the expansion of the buffer into the backfill (Gunnarsson et. al, 2004). SKB did not believe that such a contradiction existed and suggested that an increased density would be beneficial for both these aspects of the backfill performance.

Flow along tunnels and deposition holes will be influenced by the buffer and backfill as well as by the rock within the excavation disturbed zone (EDZ). SKB was asked to clarify whether the EDZ needs to be considered in conjunction with the definition of the function indicators for the buffer and backfill. SKB suggested that the EDZ is much less critical than the backfill performance, so that flow and radionuclide transport related to the EDZ is of limited significance.

Table 3. SR-CAN table of Function Indicators, with associated Criteria, for backfill.

Function indicator	**Criterion**	**Rationale**
Backfill in deposition tunnels		
Compressibility	$M^{Backfill} > 10$ MPa (M = compression module)	Limit buffer expansion
Hydraulic conductivity	$k^{Backfill} < 10^{-10}$ m/s	Limit advective transport
Swelling pressure	$P_{Swell}^{Backfill} > 0.1$ MPa	Ensure homogeneity
Minimum temperature	$T^{Backfill} > 0°C$	Avoid freezing

4. Material selection

Material selection for the buffer and backfill must take into consideration the long-term performance of these materials, and this requires evaluation of many material properties, especially for the buffer. However, diversity of suppliers must also be considered in order to avoid reliance on a single supplier during a period of several decades. Access to several suppliers may also be favourable from a cost perspective. MX-80 bentonite has been used as SKB's reference material for the buffer since the KBS-3 concept was first proposed, and the reference material for the backfill is a mixture of MX-80 bentonite and crushed rock (in proportions 15:85 or 30:70). SKB is now looking into alternative materials.

SKB's contractor (Clay Technology AB) presented information on the various types of bentonitic materials that are being evaluated for buffer and backfill. SKB stated that tri-octahedral clays are not completely ruled out of consideration for buffer/ backfill, but that the great majority of information is on di-octahedral clays. Around 20 materials are being examined, but most results presented were related to three sources of bentonite that are currently extensively analyzed:

- MX-80, Wyoming, US
- Deponite CaN, Milos, Greece
- Friedland ton, Mecklenburg, Germany

SKB believes that the criteria for materials selection should be based on a detailed understanding of the correlation between mineralogy and desired properties (i.e., meeting function indicator criteria), rather than defining a specific source of bentonite.

Accordingly, SKB is conducting an extensive suite of tests to characterize the properties of the three bentonites noted above. Characterization tests on purified samples include mineral composition, elemental composition and ion-exchange properties. Mineral composition has been analysed by powder X-ray diffraction (XRD; qualitatively and quantitatively) and elemental composition by inductively coupled plasma atomic emission spectroscopy (ICP/AES), as well as IR LECO (sulphur and carbon analyses). Cation exchange properties were analysed by use of NH_4^+ (total amount of exchangeable ions) and Cu^{2+} (CEC). The exchanged ions were analysed by ICP/AES and structural formulas for the materials were derived. Pure ion exchanged clay fractions (Na and Ca) were synthesised based on the raw materials.

SKB's contractor, Clay Technology AB, is conducting a series of performance tests on the three bentonite sources noted above. The objective of these tests is to evaluate the effects of mineralogical properties (e.g. content of exchangeable cations, montmorillonite charge, content of non-clay minerals, and CEC), density and salinity on the following function indicator criteria for the buffer and backfill:

- swelling pressure,
- hydraulic conductivity,
- diffusion,
- rheology.

Figure 2. Sun drying of bentonite at the Greek island Milos, which is one of the largest producers in Europe. The material Deponit CaN (Silver & Baryte Ores Mining Company) originates from this facility.

An extensive database has been developed for three bentonites thus far, and results indicate:

(1) that bentonites having broadly similar compositions, such as MX-80 and the Milos bentonites (both containing about 80% montmorillonite), display nearly equivalent isolation properties at equal cation composition, and

(2), distinctly different isolation properties of the Friedland clay can be readily interpreted based on differences in mineralogy between this material and the other reference materials.

SKB had at the time of the workshop not completed the diffusion and rheology tests.

The workshop participants were in general impressed by the data that SKB recently have gathered in the characterisation of bentonite clays and in particular the progress with alternative bentonites (other than MX-80). It could be an important advantage if SKB could develop general models for bentonite, rather than being tied to only a single "reference material".

A general issue that SKB should address is the unavoidable discrepancy in the amount of characterization data that is available MX-80 compared to the other bentonites. MX-80 has for instance been used in all large scale tests that have been conducted so far. SKB's general attitude is that bentonites of similar smectite content will behave in a similar manner with respect to function indicator criteria. SKB plans to use a mineralogical basis by which to compare and establish the equivalence of different bentonites that might be considered for buffer and backfill. While it is not impossible that SKB will use different bentonites for buffer and for backfill, it is more likely that one source material will be selected for both.

Workshop participants agreed with SKB that smectite content could be a useful basis for selecting bentonites for use as buffer and backfill materials, but that more work may be needed to ensure that any such basis was scientifically justified. It was suggested, for example, that bentonites with different proportions of accessory phases in addition to the predominant smectite clays might display some different behaviour. It was recommended that SKB should in particular conduct field-experiments with alternative bentonites over time scales that are as long as practically achievable. SKB announced that such experiments are indeed planned for alternative bentonites (e.g. experiments corresponding to the long-term buffer experiments at the Äspö Hard Rock Laboratory). There is a need to further confirm SKB mineralogical approach to establishing consistency among different bentonites. SKB was also reminded that introduction of contaminants within backfill materials has to be considered, since even a small content may in the end, when all tunnels have been backfilled, correspond to a large amount.

Material selection will involve other components in addition to buffer and backfill. Although not part of the workshop’s main theme, the basis for selection of low-alkalinity cements for use as possible sealing and grouting materials in a KBS-3 repository was brought up. A concern that was expressed is that these materials may contain additives that could influence long-term performance in a manner which is difficult to predict.

5. Early THM-evolution

5.1 Overview

The early Thermal (T)-Hydrological (H)-Mechanical (M) evolution of the buffer and backfill soon after canister emplacement and tunnel backfilling involve:

- heat transport by conduction and convection,
- moisture transport,
- gas phase flow,
- mechanical evolution.

Relevant issues that must be considered during this time include the evolution of maximum temperatures in various parts of the EBS, resaturation processes (e.g. drying close to the near the canister) as well as the effects of uneven wetting and redistribution of buffer material due to swelling. To address these issues SKB are working with mathematical models, and large-scale experiments to evaluate and confirm modelling results, and small-scale experiments mainly to determine material properties and parameters needed for the modelling. The main challenge in predicting early THM evolution is the coupled nature of the processes involved.

SKB presented their program on evaluating coupled THM processes, with emphasis on their field-scale, high-temperature TBT experiment at the Äspö Hard Rock Laboratory (see Figure 3). The TBT tests are used to evaluate processes during the early thermal and re-saturation period, including conductive and convective heat transport, gas and moisture transport, and the evolution of mechanical stresses. Layers of bentonite and sand as well as bentonite alone are being heated in a controlled manner. The measured evolution in temperature, relative humidity (RH), total pressure, pore pressure, cable forces and deformation of metal components are compared to model predictions as a basis for performance confirmation.

SKB presented results from a series of sensitivity studies on the hydration behaviour of bentonite (MX-80) buffer in a KBS-3 type repository at elevated temperature. The objective is to find the relative importance of conditions and factors that will control the time-scale for re-saturation of the bentonite buffer during the early thermal period (i.e. coupled T-H processes). Factors explicitly considered in the model calculations (using Code_Bright) included buffer thermal conductivity as a function of saturation, buffer suction as a function of saturation, intrinsic permeability of the buffer, groundwater pressure, water and moisture fluxes, tortuosity of the buffer, variability in power characteristics of the emplaced spent fuel, and initial saturation of the as-emplaced buffer.

Calculation results to-date, illustrated by Figure 4, suggest that hydration of the buffer is expected to be completed within 2 to 4 years for most assumptions regarding buffer properties. Suction and intrinsic permeability of the buffer material are found to be the most important parameters affecting hydration time. A conservative but reasonably realistic bound of 10 years is estimated for full hydration of the buffer (assuming that a fixed groundwater pressure is maintained at the interface between the buffer and the rock wall). Calculations indicate that vapour flow, as controlled by lower tortuosity, is important for the initial de-saturation close to the canister surface, but relatively unimportant for the hydration time. SKB suggested additional code development is required, and that in subsequent applications the code will consider mechanical aspects and initial inhomogeneities in the buffer.

Workshop participants asked if SKB had evaluated the possibility of a heterogeneous resaturation of the buffer and, if so, whether there are any associated adverse consequences. SKB stated they had both modelled and experimentally studied this issue, but found that heterogeneous re-saturation would not lead to any significant consequences. Although some buffer inhomogeneities can remain in the buffer due to friction in the clay, these are acceptable and will not affect the buffer function. Large-scale tests on buffer material outside of Sweden (e.g. FEBEX) also support this contention.

Workshop participants asked if separation of bentonite and crushed rock could occur during the resaturation of the backfill. SKB are currently studying this issue. If blocks of backfill material are prepared, separation is minimized.

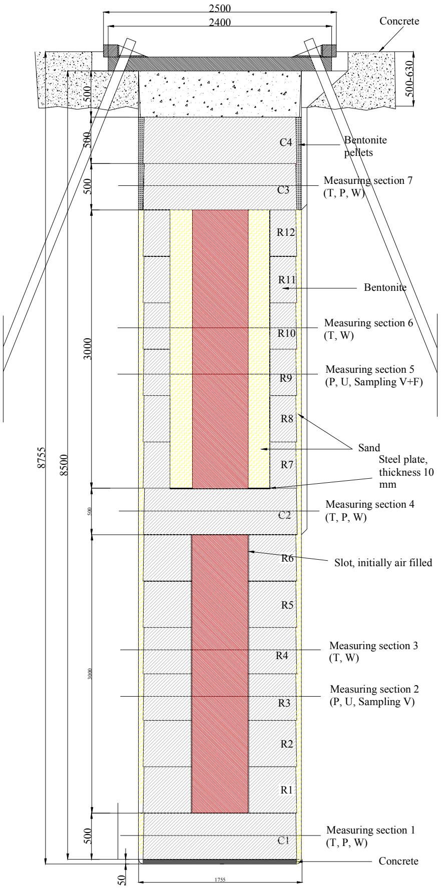

Figure 3. Configuration of the Äspö HRL TBT (Temperature Buffer Test) experiment on THM processes

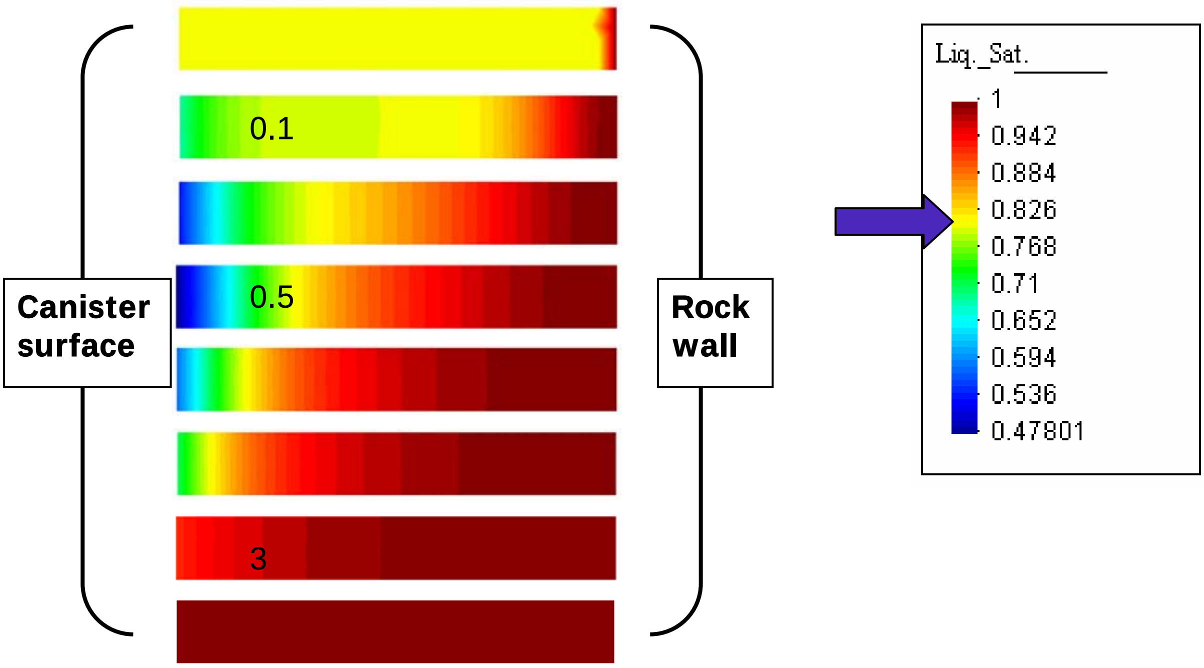

Figure 4. Resaturation of bentonite buffer. The colour bars correspond to the buffer thickness. The left side corresponds to the canister side and the right corresponds to the rock wall side. The evolution of the resaturation is illustrated by progressing downwards in the figure (the numbers 0.1, 0.5 and 3 on the left hand side done elapsed time in years). The numbers within the box on the right hand side (which correspond to the colours in the figure) denote degree of saturation. Note the initially decreasing water content near the hot canister surface after about half a year (source: SKB workshop presentation).

5.2 Extremely long resaturation times

SKB discussed factors that could delay buffer resaturation over timescales as long as hundreds of years, and associated consequences for the long-term behaviour of this barrier. At this time, the only experimental data that might shed some light on this issue are from the TBT tests. There are plans, however, to also evaluate data from the Äspö Prototype Test. Preliminary evidence from this test suggests that re-saturation times may be much longer than a few years. It was noted that the intrinsic permeability of bentonite-based materials could decrease with time, leading to longer than expected re-saturation times. This observation was countered by SKB's observation that suction, a more sensitive parameter with respect to re-saturation, did not appreciably change with time.

Workshop participants were concerned that extremely long resaturation times could be detrimental to long-term buffer performance. However, SKB noted it did not have a maximum allowable time for re-saturation, and that delayed re-saturation on the order of 1000 years could even be beneficial to waste isolation. Extremely dry deposition holes, possibly attributable to low permeability and unfractured nature of the surrounding rock, could be the rate controlling process for re-saturation of the buffer and backfill in some cases. In such cases, transfer of dissolved species between the rock and the buffer would be extremely small, which in principle would be advantageous from an isolation point of view. However, SKB emphasised that ventilation and transfer of gaseous components in a continuous pathway would not be acceptable. Ventilation would imply loss of liquid water due to vaporization and concentration of solutes in the residual liquid, which could lead to some accumulation of salts near the canister surface. In the absence of such transport, SKB noted that the amounts of available gas and dissolved solutes would be similar regardless of whether resaturation is slow or fast. Workshop participants felt that at least scoping calculations would be needed to provide an upper limit for the amount of salt accumulation. A potential role for convection cells (heat-pipe effect) leading to salt accumulation at the canister surface was suggested.

5.3 Adding chemical processes to THM-modelling

Workshop participants noted that chemical effects (C) were not considered in SKB's T-H-M models. Such effects are known to adversely impact certain mechanical properties of bentonite-based barriers, such as the swelling pressure, and could also cause the barriers to become lithified due to cementation of clay minerals and accessory phases leading to fracturing. This raises questions regarding SKB's assertion, noted in the preceding section, of no adverse impacts due to long re-saturation times, because chemical processes may be particularly important during resaturation due to the elevated temperatures in the near field. SKB suggested that such issues will be addressed in the upcoming SR-Can safety assessment. However, SKB insisted that no code exists for full T-H-M-C coupling and that the proper approach was to partially de-couple the relevant processes and evaluate them separately. SKB noted, for example, that there is no quantitative basis for evaluation of the M-C coupling and that such effects would have to be addressed using expert judgement rather than modelling. In addition, SKB plans to evaluate cementation processes in the context of the LOT-experiments at Äspö HRL.

Some workshop participants felt that SKB is overly pessimistic regarding the possibility of integrating chemical effects into T-H-M modelling. Certainly some codes do exist that link chemistry into T-H and even T-H-M models, such as TOUGHREACT. Furthermore, it is clear that simpler, but possibly incomplete, studies on T-H-M coupling alone fail to incorporate known chemical processes (e.g. Couture effect). One suggestion was that SKB could, as an intermediate step, explicitly couple groundwater salinity (and its known effects on swelling pressure) into THM-modelling of the buffer and backfill.

Avoidance of including chemical processes in T-H-M models has long been defended on the basis that it is difficult to do, but not that it is unnecessary to do. At this mature stage of its program, it would be helpful if SKB could clarify whether it plans to use an uncoupled analysis of chemical processes, or whether it plans to attempt a more difficult but not impossible task of complex T-H-M-C modelling to evaluate known coupled effects. As an alternative, SKB might engage on a number of long-term tests to empirically address potential T-H-M-C coupling. It is not clear that such tests could be completed in a reasonable time scale.

5.4 Influence of slots and gaps

SKB presented a review of T-H-M processes that may arise within the initial gaps and cracks of as-emplaced buffer and backfill. Of particular concern are gaps between the buffer and canister (which affect the thermal evolution of the waste package and near field) and gaps between the buffer and rock (which affect buffer re-saturation and associated mechanical and chemical processes discussed in the preceding section). At this time, SKB's view is that after saturation and homogenisation all gaps and cracks will be sealed. Density gradients due to friction will remain, however, especially in the transitional area between the buffer and backfill. SKB believes that the processes are well-known on a conceptual level, but that quantitative numerical models of the strongly coupled T-H-M processes involved are only approximate, especially for initially unsaturated conditions.

SKI's consultants raised a number of questions. It was noted that heat-transfer via moisture/ vapour transport could also be important, and that SKB seems to be considering this process in addition to radiative heat-transfer. SKB noted that any gap between the buffer and rock was relatively unimportant to initial heat-transfer calculations. Any persistent gap between the canister and buffer, however, would sensitively affect near-field thermal evolution up until the time the gap closed. Conductive heat-transfer would thereafter dominate over radiative heat-transfer. SKB mentioned that their current approach to concerns about low-density regions attributable to initial gaps is to over-densify the buffer, such that the final bulk density of the buffer when fully water-saturated would meet the adopted function indicator criteria.

It was suggested that gaps could in certain cases persist in spite of the development of the swelling pressure. SKB responded that this behaviour would not be consistent with their conceptual model for bentonite performance.

5.5 Temperature limit

Temperature limits for the buffer were also discussed. The initial temperature of an as-emplaced canister is estimated to be about 90˚C. SKB wants to keep temperatures within the buffer below boiling to minimize the deposition of residual salts. It was noted, however, that (1) some concentration of solutes could occur by evaporation of bentonite porewaters at below-boiling temperatures, and (2) there is known to be significant dissolution/precipitation of accessory minerals in bentonite buffers driven by a temperature gradient, even at sub-boiling conditions. Thus, SKB's estimated temperature of 90˚C for the buffer seems somewhat arbitrary, possibly potentially ineffective in eliminating coupled T-C effects, and possibly overly restrictive with respect to possible optimisation of repository design and operational safety.

6. Effects of salinity

SKB is collaborating with POSIVA on the significance of groundwater salinity for buffer and backfill performance. The most important justification for addressing saline conditions is the intrusion of saline groundwater, an event that could be associated with future glaciations. In addition, upconing of highly saline groundwater (during open repository conditions) and salt deposition in the buffer during the resaturation phase (due to evaporation) may also occur.

The trend of decreasing bentonite swelling pressure with increasing salinity is well known and has been studied for several decades. It arises mainly from ionic-strength effects on the osmotic pressure of water between clay particles and from the effects of varying ionic compositions on the hydration potential of interlamellar spaces within these particles (Pusch, 2002 - SKB TR-02-20). Nevertheless, SKB pointed out that the effects of increasing salinity on swelling pressure is small at planned buffer densities near 2000 kg/m^3 (Figure 5). SKB has recently extended studies of bentonite swelling as a function of salinity to include alternative bentonites (i.e., other than MX-80).

SKB previously used diffuse double-layer theory to explain the influence of salinity on swelling pressure. A comparison between model predictions and experimental results suggested a need to re-evaluate this concept. However, a recently developed application of the semi-empirical Donnan model provides a very good agreement (Figure 5).

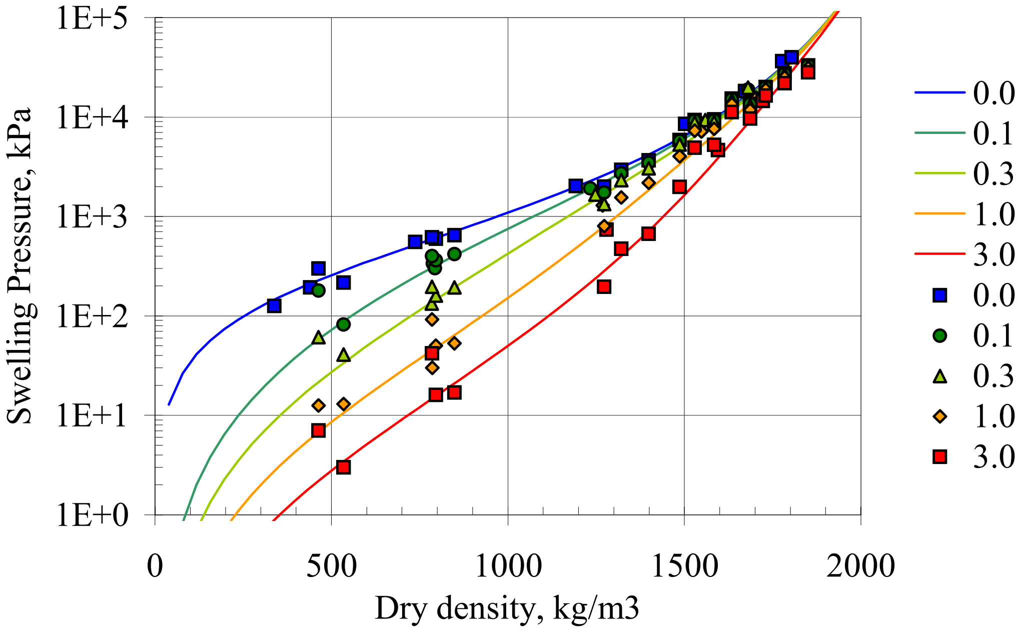

Figure 5. The effect of increasing salinity, from 0 to 3.0 M NaCl, on swelling pressure of bentonite as a function of dry density. Symbols represent experimental measurements and lines represent model predictions using the semi-empirical Donnan model (source: SKB workshop presentation).

Workshop participants requested that SKB provide additional clarification regarding the criteria for maximum salinity (Table 2). SKB explained that the 100 g/l criterion is based on a desire to avoid, if possible, ingress of extremely saline shield brines into the repository environment. In terms of actual effects on swelling pressure, however, the 100 g/l is somewhat arbitrary in SKB's view. SKB noted that this threshold is far lower than the unrealistically high 3 M NaCl solution used to investigate salinity effects. The lower 35 g/l criterion for the backfill is needed because the bentonite density will be lower in the backfill. SKB acknowledged that the high salinity limit is a key issue in the context of future work on backfill design. SKB may re-evaluate the justification for both criteria in the future.

Workshop participants asked whether SKB had analysed implications of cyclic changes in salinity from very low to high during a glacial cycle. SKB do not anticipate any adverse effects in connection with such cycles. It was noted that the swelling pressure response from a change in salinity is a reversible processes. SKB's position is that sufficient swelling pressure and proper functioning of buffer and backfill should be maintained as long as the density function indicator criterion is maintained.

Another issue that was brought up is whether groundwater salinity issues may influence the KBS-3 emplacement orientation and/or backfill specifications. SKB mentioned that field data from SKB's Plug Test suggests that 30:70 backfill mixtures of bentonite and rock are barely adequate to meet engineering and function indicator criteria up to moderately saline conditions. SKB is evaluating alternative engineering changes to improve performance, e.g. a finer grain size for crushed rock and use of pre-compacted blocks of bentonite. The horizontal emplacement option (KBS-3H) is also currently being investigated.

Other indirect buffer and backfill influences related to salinity were also considered and are discussed in Sections 7 and 8.

7. Chemical alteration of bentonite

Favourable properties of emplaced buffer and backfill must be maintained over extremely long periods of time. In the safety assessment context, it should either be shown that feasible chemical processes occur to a negligible extent and can be disregarded, or that they do not cause an extensive degradation of buffer and backfill performance. SKB suggested that a main problem in this regard is that alteration processes may be so slow that it is difficult, if not impossible, to study them experimentally. Examples of such processes are:

- redistribution/enrichment of accessory minerals such as calcite and gypsum during the early non-isothermal period of repository evolution,
- enrichment of substances from groundwater (e.g. $NaCl$, $CaCl_2$),
- montmorillonite transformation to non-swelling minerals such as illite or chlorite, and,
- montmorillonite dissolution.

SKB analyses these processes based on experimental studies of mechanisms, large-scale long-term tests, accelerated tests, mathematical modelling and natural-analogue studies. In addition, fast processes such as montmorillonite inter-lamellar reactions are studied.

SKB focussed in particular on establishing a technical basis for excluding illitisation (Figure 6), a process which would convert the bentonite to an essentially non-swelling material. According to experiments and natural analogue studies, the activation energy for the reaction montmorillonite-to-illite is such that a temperature approaching 100°C is needed for this reaction to occur to an appreciable extent over a period of 10^6 years (Figure 7). It should be noted that in a real repository appreciably elevated temperature is only expected for a very limited period of the total 10^6 years addressed in safety assessment.

Of particular note are SKB's "Long Term Test of Buffer Material" (LOT) tests in which full-scale waste packages have been emplaced into rock deposition holes. By including heaters and instruments to monitor re-saturation, SKB expects that further information (performance confirmation) will be obtained to further validate their modelled predictions of negligible illitisation of smectite.

With respect to chemical effects on buffer integrity, several questions were posed to SKB by workshop participants. SKB asserted that kinetic reaction rates, not transport of K^+ and Al^{3+} ions, would be the rate-limiting step for possible long-term illitisation. While uncertainties were acknowledged with respect to transition-state parameters within its models for the rate of illitisation, SKB feels that laboratory and natural analogue data provide sufficient bounds to such parameters that they are confident the rates will be acceptably low, perhaps even negligible. However, a comment made during the first day of the workshop was that conversion of montmorillonite to beidellite would occur under high-salinity conditions. Beidellite would in turn be converted to illite. In order to handle this, SKB may consider assuming that the rate of smectite conversion only to be dependent on the mass transfer limitation for supply of dissolved potassium in groundwater rather than the reaction kinetics.

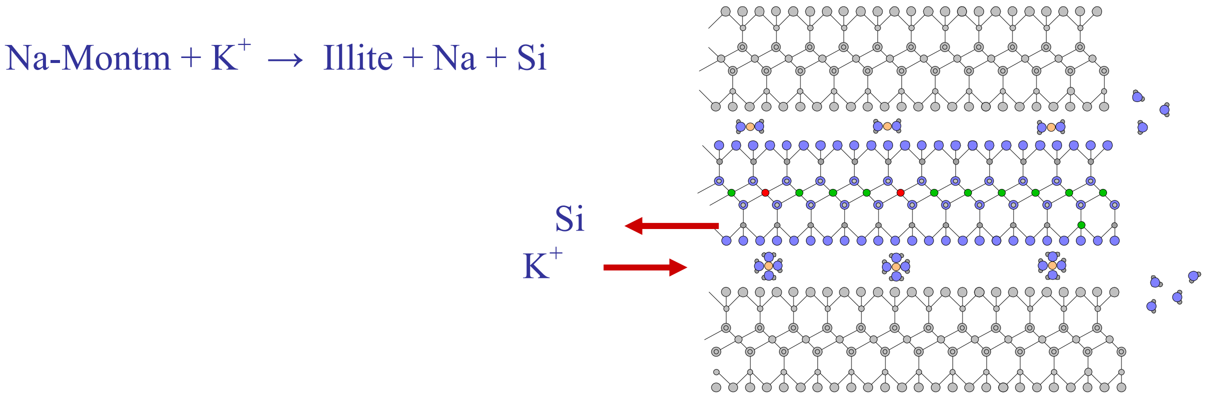

Figure 6. Layer structure of montmorillonite clay allowing entry of water and dissolved species, as well as "swelling" of overall structure. The simplified stochiometric equation and the mass transfer arrows denote illitisation, which is perhaps the most well-known chemical alteration of bentonite.

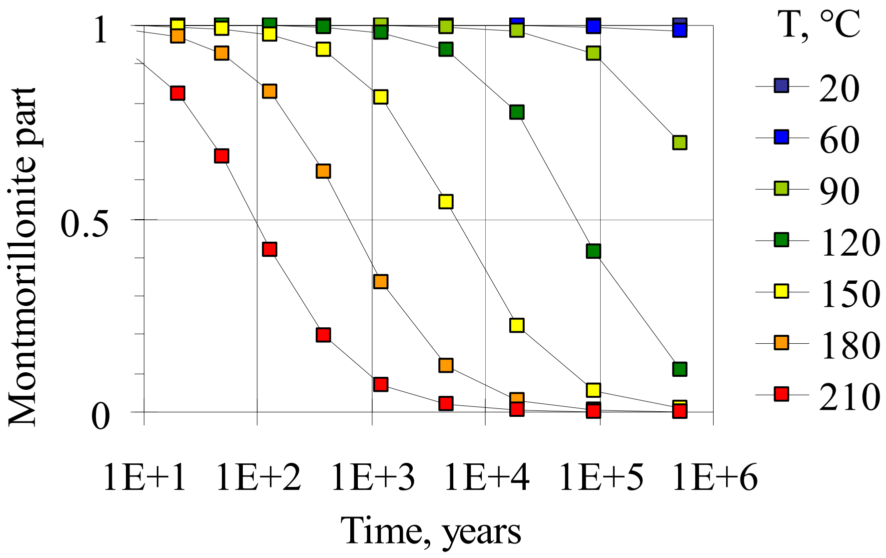

Figure 7. Fraction which is altered from montmorillonite to illite according to a model by Huang et al. 1993 (using the following parameters: A = 8.5 E+4 L/s/mole, Ea = 115 kJ/mole, {K+} = 0.01 mole/L).

It was noted that the SKB presentation did not in detail address other possible chemical processes that might degrade or compromise buffer function indicators, such as re-distribution of accessory phases in a temperature gradient leading to localized 'sealing' and loss of swelling of smectite. These will likely be issues on which SKI will seek further discussion with SKB.

SKI's consultants asked what activities were being planned by SKB for the possible use of low-pH cements in the SFL-2 repository. While some adverse effects of high pH on the stability of smectite in bentonite were acknowledged by SKB, it was suggested that an upper limit of pH 11 would provide a margin, below which unfavourable interactions between bentonite and cement would be avoided. SKB did not provide any conclusive justification for this statement, but noted that some support for their position could come from work on the EC-project ECOCLAY. More work is likely to be needed to justify and defend requirements on cements used in the vicinity of the repository environment. A relevant context is e.g. grouting of deposition holes. In addition to the known effects on smectite stability, there may also be other impacts which must be considered, e.g. on copper canister corrosion due to higher pH than ambient groundwater. It was noted that other repository programs in Finland, Japan and elsewhere are also studying the issue of high pH on smectite stability, as well as the development of lower pH grouts.

Workshop participants asked whether SKB planned to develop a more comprehensive basis for evaluating the thermodynamic stability (and theoretical solubility) of the smectite clays relative to temperatures, temperature gradients and fluid compositions that could exist in the near field. It was noted that SKB presently accounts for the possible transformation of smectite (of unspecified composition) to illite using a kinetic model. Workshop participants wondered, however, whether a more complete understanding of smectite's known solid-solution behaviour would provide a robust, thermodynamic basis for assessing the stabilities of these minerals in relation to variations in their chemical composition, the compositions of coexisting buffer porewaters and temperature. SKB noted that future studies were being planned to investigate the stabilities of the smectite clays and other buffer minerals.

8. Piping/erosion

Several of the key safety features of the buffer and backfill depend on a long-term maintenance of sufficiently high bentonite density (Table 1 and 3). SKB has identified two processes related to the loss of bentonite:

- piping followed by erosion before repository closure,
- erosion of colloidal clay into flowing fractures after closure.

Piping can occur in both the buffer and backfill, but only at high water pressure gradients and high water flow rates (i.e. before or soon after deposition tunnel closure). Piping has the potential to lead to significant loss of bentonite, hence, possibly significant degradation in buffer and backfill performance. Most likely this condition will arise at the intersection of highly conductive, water-bearing fractures, which makes the buffer in the KBS-3 horizontal orientation somewhat more susceptible to piping than in the KBS-3 vertical orientation. Erosion occurs when the drag forces on the particles are higher than the sum of the friction and attraction forces between the particles and the structure (exceeding a critical shear stress).

Two sets of tests are being conducted by SKB on this topic: the ongoing KBS-3H (buffer) tests and the recently started Backfill and Closure Project. The tests for KBS-3H have been done at laboratory scale, 1/10 full scale and full scale. Different configurations of water in-flow and out-flow conduits have been used, and both pressure-control and flow-controlled conditions have been employed. Figure 8 summarises these results.

Interpretation of the test data is complicated by effects arising from flow rate, water pressure, orientation of the inlet/outlet, length of piping channel, physical characteristics of the buffer/backfill and groundwater salinity. A change in salinity from 0 to 1.1%, for example, led to an almost 10-fold increase in piping erosion rate at a fixed flow rate.

SKB recognises the importance of this issue, and is actively working to further explore and evaluate factors that may mitigate piping. Favourable hydraulic properties of the host rock, as well as specific operational procedures (rapid sealing of deposition tunnels) may attenuate the severity of piping.

The potential deleterious effect of piping on buffer and backfill performance was thoroughly discussed. Piping may occur prior to full re-saturation of the buffer or backfill, but may be terminated once emplacement drifts are sealed. Hence, operational plans and methods will be important factors in addressing this issue, including excavation, rate of waste package emplacement, and sealing of deposition drifts. Initial gaps between buffer and rock, as well as the canister, may have important roles in the occurrence of piping, but this is not clear and more studies are planned by SKB. Furthermore, there must be some “sink” for bentonite removed by piping.

SKB is conducting further investigations on the rate and potential duration, hence magnitude, of piping in both laboratory and planned field tests. SKB suggested that piping/erosion could possibly be handled by engineering measures, but may also have to be accounted for explicitly in safety assessment by, e.g., mass-balance calculations (presumably by keeping track of the amount of lost bentonite). Furthermore, it was suggested that the potential for piping might be a criterion for selecting and rejecting rock suitable for deposition tunnels. Use of grouts to attenuate fracture flow may be used, but might not be feasible if located too close to the buffer due to potential effects of hyperalkaline pore fluids on bentonite stability. Apparently no other repository program is yet evaluating this issue.

SKB and workshop participants did not address the possible erosion of colloidal clay from the buffer into flowing fractures long after closure. This issue should be discussed within another context.

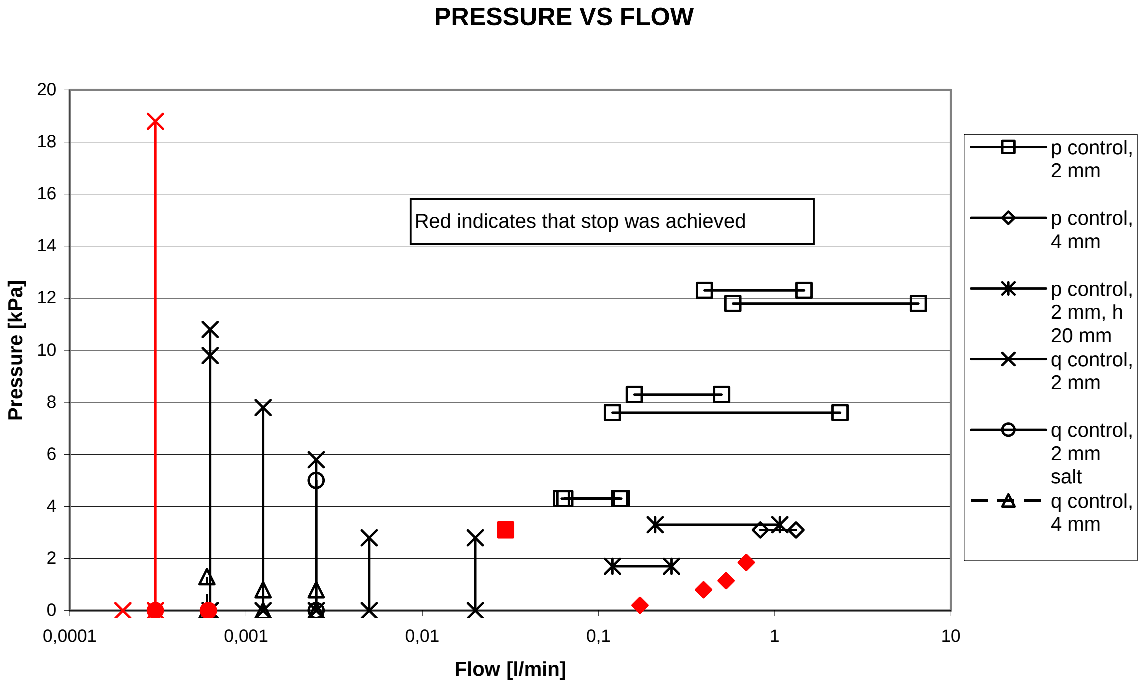

Figure 8. Data from constant-flow (q) and constant-pressure (p) tests on piping. Red symbols indicate where piping did not occur or was rapidly blocked (source: SKB workshop presentation).

9. Permafrost

SKB addressed two interrelated processes that may occur during potential freezing of buffer and backfill:

- in fine-grained materials, formation of ice-lenses takes place at temperatures below zero,
- consolidation effects of clay structures may occur when subjected to constrained (i.e., rigid) boundary conditions.

In the former process, water is drawn into pores of fine-grained material at temperatures below zero, where it freezes as an “ice lens” Ice lenses can continue to grow as long as water is present and the temperature is below freezing. For unconstrained boundary conditions, continued formation of ice lenses can lead to frost heaves. For constrained, rigid boundary conditions, SKB estimates that formation of such lenses will result in a pressure increase of about 3 MPa for each degree of temperature below-freezing. This pressure increase under constrained conditions will cause in redistribution of unfrozen water due to consolidation of the host material. This pressure increase will also be applied to the rock interface and any canister embedded within the buffer as it freezes. The fraction of frozen water as a function of temperature needs to be investigated.

If and when the ice lens thaws, the residual material will have increased hydraulic conductivity, and possibly fractures, attributable to this consolidation process. It is not clear whether such permeability changes and damage will be permanent, or whether subsequent re-swelling of a thawed buffer will heal fractures and zones of higher hydraulic conductivity. In the backfill, there may be an increased hydraulic conductivity after freezing and thawing along the buffer/rock interface and within the backfill itself. There may be a segregation of materials.

During the question period, a number of points were discussed. SKB noted that freezing may be an issue in “shallower” parts of a planned repository, taken to be a depth down to 300 meters below ground surface, over which a glacier might form. SKB further noted that freezing would also likely lead to formation of highly saline waters near the freezing front, and even possible precipitation of salts. At this point, SKB is assuming that if any part of the buffer were to freeze, canister integrity could not be assured. This is a conservative, possibly overly pessimistic assumption, and SKB continues to evaluate its position on this issue. It was noted that avoidance of freezing could force SKB to seek a deeper repository position. This option could, however, conflict with site constraints arising from in situ stresses and stress anisotropy.

10. Canister sinking

The issue of canister sinking has been addressed by SKB since the early 1980's through both experimental and theoretical approaches. The potential process is divided by SKB into three parts:

- consolidation/swelling caused by force imbalances on the pore water
- differences in volumetric creep below and above the canister, and
- deviatoric creep caused by shear stresses.

Of these three possibilities, the latter is expected to be the most problematic to address. The long-term creep behaviour of the buffer is assumed by SKB to follow the Singh-Mitchell creep model developed for soils, although SKB acknowledged that validation of such a model over long time periods is difficult. In SKB's model, an initial period of consolidation occurs in the first approximately 300 years, followed by longer-term creep. All calculations indicate that the amount of canister displacement is expected to be small (several millimetres), and may indeed involve an upward displacement. SKB acknowledged that long-term deviatoric stress on the canister from the buffer may lead to a decrease in friction angle. However, the friction angle would have to decrease from 10˚ to 0.7˚ for the buffer to plasticize sufficiently to allow the canister to sink to the bottom of a deposition hole, conditions which seem highly unlikely.

A number of questions and comments were raised by this presentation, partially because SKB had not suggested any function indicator criterion, as noted earlier. The key question was at what density canister sinking might become a problem within the context of SKB's conceptual model. This value has not been calculated by SKB. Workshop participants acknowledged the need for a formal criterion, but did not expect canister sinking to be a probable scenario.

Given the acknowledged difficulty in confirming and validating extremely slow creep behaviour for the buffer, SKB was asked if there were alterative methods and supporting studies that might be conducted. For example, other clays or non-clay materials might be tested to confirm the general applicability of the Singh-Mitchell creep model over extended time scales. Natural analogues might be sought (e.g., sinking of dense, high-pressure tectonic blocks within pelitic (clay) melanges to examine sinking over timescales far beyond those practical in laboratory or field tests. Centrifuges have been used in the past to generate accelerated g-force (whole body acceleration entirely equivalent to gravity) to study the sinking of waste containers in pelagic muds during ocean disposal studies in the 1980's. SKB noted that it has considered a wide range of test conditions to test its conceptual model. Furthermore, many natural analogue or centrifuge studies may be more appropriate to evaluating initial consolidation rather than long-term creep.

11. Concluding discussion

On the third and final day of the Workshop, SKI and its technical contractors met to discuss the presentations and answers to questions made by SKB regarding issues on the buffer and backfill. Each participant was asked to briefly summarize their key points. The issues ranged from those considered uncertain, possibly requiring substantial new efforts, to those only requiring modest additional information and clarification from SKB. No clear judgments were made concerning the relative importance of a particular issue to safety and regulatory compliance. In subsequent review work attention must be given to such a ranking of issues and also when an issue needs to be resolved within the context of an extended licensing process. Moreover, there is a need to establish a method by which SKB and the Swedish regulators (SKI and SSI) can reach concurrence that sufficiency of information (as opposed to the impossible-to-achieve “complete understanding”) on any specific issue has been achieved.

A general observation by all Workshop participants was that the open access and forthright discussions by SKB and its contractors in such technical workshops was greatly appreciated and should assist the preparation by SKI to receive and review license applications from SKB in a timely manner.

11.1 Opinions related to SKB’s presentations

The following section examines the opinions of SKI and its contractors related to the key issues brought up by SKB at the Workshop.

The function indicators concept was regarded as a potentially useful novelty in SKB’s safety assessment approach. However, there were concerns related to the derivation of the list of indicators, the completeness of this list, the basis for deriving specific quantitative criteria for each function indicator, and relating function indicators directly to safety assessment. Participants felt impacts on repository safety and regulatory compliance should guide the selection of function indicators and associated specific criteria values. Treatment of uncertainty within the function indicator concept, explicit uncertainties in data and conceptual models, and the propagation of such uncertainties into long-term safety assessments of the buffer and backfill was also raised as an issue in which more information is needed.

Participants praised the ongoing systematic gathering of data on swelling pressure, density, permeability, and salinity effects relevant to the performance of the buffer and backfill, notably through the work of Clay Technology AB. The amount of data already collected on alternative bentonite sources is particularly impressive. If this work is continued, SKB may confidently develop general models for bentonite rather than being tied to only a single “reference” material.

The thermal-hydrological (T-M) modelling by SKB was also judged to be excellent. However, participants look forward to SKB’s treatment of a wider array of initial properties and boundary conditions to explore re-saturation of buffer, especially cases that might lead to extremely long (>100 years) re-saturation. SKB's analysis of the impact of gaps on re-saturation and repository heating were good starts, but do not seem to provide a sufficient range of boundary conditions. In particular, the persistence of such gaps, rather than assumed sealing of such gaps, may lead to a complex evolution in thermal, hydrological, mechanical and chemical conditions. The consequence of long delays in re-saturation (on the order of 1000 years) may or may not be favourable to repository performance; a more compelling analysis of this situation, either by bounding analysis or detailed coupled process modelling, is warranted.

Related to this potential issue of gaps is the potential issue of interfaces. Rock-buffer and canister-buffer, in particular, are two interfaces that may impact overall repository performance and safety. Data from field tests on assembled EBS and rock systems may provide crucial information that may confirm or refute laboratory data developed on single components. At this stage before completion of long-duration field tests, SKB is encouraged to examine a wider range of possible boundary conditions and assumptions in their models and laboratory tests regarding the continuity of T-H-M-C processes at such interfaces.

It was also recommended by Workshop participants that SKB should further consider salinity effects on the buffer and backfill. Both glacially driven cyclic changes in salinity of host rock groundwater and freeze/thaw concentration effects need a deeper level of analysis by SKB before they can be confidently excluded as adverse events.

Illitisation models for montmorillonite appear to be well conceived, with defensible lines of evidence to support SKB's contention this will not be an issue with respect to long-term repository safety. However, certain other chemical interactions are not equally well established, e.g. if cements or grouts (and associated hyperalkaline pore fluids) were placed in proximity to either the buffer or backfill. Moreover, cementation of the buffer, driven by re-distribution of soluble accessory phases during the initial period of high thermal gradients is considered to be an issue not fully evaluated yet by SKB. Loss of swelling and lithification are but two potential consequences of this process. There may be ways to bound the occurrence, rate, magnitude and extent of such cementation, but SKB has not yet presented a program to address these factors. Application of fully coupled T-H-M-C models to this problem, and possibly others related to the early non-isothermal evolution of the near field, may be a useful complementary approach to help bound these parameters. Workshop participants suggested that SKB might in a general sense benefit from using more comprehensive approaches for the representation of T-H-M-C couplings.

Potential piping and erosion are concerns that SKB must address, given the possible adverse consequences to assuring isolation. SKB's program is appropriately balanced between further laboratory tests, as well as consideration of design and operational factors that may mitigate the occurrence or duration of piping. The KBS-3H concept seems particularly vulnerable to this process. Use of a sealed container for package and buffer emplacement, rather than the current wire mesh design, might obviate any potential piping until the period that emplacement drifts are sealed.

11.2 Other opinions

The following section examines other relevant opinions of SKI and its contractors that are indirectly related to SKB's presentations.

Site conditions and EBS performance are closely linked, each setting important boundary conditions for the other. Assuming homogenous boundary conditions for some testing of buffer and backfill seems possibly optimistic, and the validity and applicability of this assumption ought to be tested by SKB. Furthermore, there is a direct linkage between external, scenario-initiating events in the site and the long-term performance of the EBS, notably climate change and glaciation. Workshop participants suggested a more comprehensive approach is needed to account for the linkage of processes between site understanding and EBS behaviour for such scenarios, rather than separate consideration of these sub-systems. This would include consideration of asymmetric mechanical loading and unloading, heterogeneous hydraulic conditions, ambient anisotropic stress, freeze/thaw, cyclic salinity changes, high pH plumes from cement, buffer erosion, etc.

An important issue is the method by which SKB will make decisions on buffer and backfill design. Short-term laboratory tests and modelling results are available now, but these seem incomplete with respect to sampling the wide array of possible repository site conditions. Multi-year field tests will be particularly valuable as they provide both a longer time period and a larger set of volumes and surface areas to confirm laboratory data and calculation models. SKB should review the context and need for additional tests.

Certainly flexibility in design, design optimization, and consideration of operational safety are anticipated and necessary freedoms that SKB must reserve during the entire site characterization and licensing process. However, it is of importance to understand the basis and justifications by which SKB will employ such flexibility and optimization in its design.

At the process-model level of understanding, there are several issues in which it is believed that SKB should investigate further or provide multiple-lines of evidence that the issues are already resolved to the extent that they are not expected to significantly impact repository safety and regulatory compliance. A general concern that was discussed in this regard is the level of documentation and traceability of data (quality management) that SKB is implementing in laboratory and field tests.

Finally, the relationship between SKB's licensing schedule, field and laboratory data collection, design decisions (e.g. KBS-3 vertical or KBS-3 horizontal emplacement options), and safety assessment implications regarding the buffer and backfill needs clarification. SKB noted that this level information is presented in its recent Activity Plan and R&D programme. Of key importance will be to reach an understanding of what level of information will be available at what time for every issue. Clearly some information will continue to be collected for many decades even after the initial stages of licensing, and indeed, many issues cannot be reasonably resolved without such long-term data to be collected during this extended period up until a licensing decision is made on repository closure. It will benefit both SKB and the regulators to reach a clear understanding of licensing schedule, R,D&D activities and safety assessment.

12. Future work

SKI's review of SKB's buffer and backfill programme will be updated in the coming years. As described above, several of the outstanding issues related to the development of the KBS-3 concept concern the buffer and backfill. More issues would have to be introduced if the horizontal concept (KBS-3H) is selected. The review of the Sr-Can safety assessment and its supporting material in late 2006 will be the next opportunity for a formal review of the buffer and backfill. Moreover, all outstanding issues must have been addressed by the time the SR-Site safety assessment is reviewed in 2008, because this assessment will be the basis for a possible decision to construct an encapsulation plant and spent fuel repository (SFL-2). SKI and its affiliated experts should further develop their review capability and knowledge of the SKB programme prior to these events.

For future reviews, a procedure for formally grouping issues according to their safety relevance and status with respect to an eventual resolution was discussed. There are several examples of such procedures in place, e.g. the use of key technical issues (KTIs) within the US programmes and the TIL-list (Technical Issues List) used by the INSITE group (SKI's independent expert group for following SKB's site investigations).

The themes and detailed objectives of independent modelling efforts should be clearly defined, such that they can be effective as a supporting tool for upcoming reviews. Although SKI has developed and used independent modelling for many years, participants thought that emphasis should be gradually shifted from the research perspective to more clearly focus on testing SKB's corresponding modelling efforts through benchmarking exercises. An approach for this could involve initial reproduction of key SKB results, followed by an evaluation of critical assumptions and parameter combinations. It was also suggested that SKI ought to promote a closer exchange of information among its own separate consulting groups on EBS, site investigations, and performance assessment.

13. References

Gunnarsson D., Börgesson L., Keto P., Tolppanen P., Hansen J. (2004) Backfilling and closure of the deep repository. Assessment of backfill concepts, SKB R-04-53, Swedish Nuclear Fuel and Waste Management Co, Stockholm.

Huang W-L, Longo J.M., Pevear D.R. (1993) An experimentally derived kinetic model for smectite-to-illite conversion and its use as a geothermometer. Clays and Clay Minerals 41, pp. 162-177.

Pusch R. (2002) The Buffer and Backfill Handbook. Part 1: Definitions, basic relationships and laboratory methods, SKB TR-02-20, Swedish Nuclear Fuel and Waste Management Co, Stockholm.

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Appendix A: Agenda and participants

SKI Workshop
EBS – Long-term Stability of Buffer and Backfill
Lund, 2004

Monday, November 15th

(Conference room Sten Broman salen)

9.00 – 9.10	Welcome and introductory remarks Purpose of the workshop	(F. Kautsky)
9.10 – 9.20	Context of EBS workshops organised by SKI	(C. Lilja)
9.20 – 9.30	Upcoming reviews e.g. Interim SR-CAN, RD&D 04, needs & possible input and feedback	(B. Strömberg)
	International perspectives	
9.30 – 9.40	NEA activities	(Ö. Toverud)
9.40 – 10.00	EU activities	(O. Stephansson)
10.00 – 10.30	Coffee break	
10.30 – 11.00	State-of-the-Art of coupled THM within DECOVALEX projects	(J. Rutqvist)
11.00 – 11.30	State-of-the-Art of geochemical processes affecting bentonite barriers and backfill	(R. Arthur)
11.30 – 11.50	Laboratory experiments; present status, lessons learned, relevance for radwaste and pending issues	(E. Alonso)
11.50 – 12.00	Analytical tool developed by CTH	(G. Sällfors)
12.00 – 13.00	Lunch	
13.00 – 13.10	High saline water - effect on clay barriers (D. Savage)	
13.10 – 13.20	STUK:s view on bentonite & backfill issues	(J. Heinonen)
13.20 – 13.30	Overview of issues raised during previous workshops	(C. Lilja)
13.30 – 13.35	Introduction to work in groups	(O. Stephansson)

13.35 – 15.30	Parallel working group sessions start preparing questions to SKB. Chairs & rapporteurs for group 1 and 2 to be appointed	
	Coffee break during session	
15.30 – 16.25	Presentations from working groups and general discussion on questions	
16.30 – 17.00	Walk to Clay Tech, Ideon	
17.00 – 19.00	Technical visit Clay Tech, Laboratory and Big Berta experiment	
19.30	Dinner at Grand Hotel	
21.30	Chairman, working group chairs & rapporteur & SKI staff finalise questions to SKB	

Tuesday, November 16th

(Conf. room Lukas Bonnier salen)

9.00 – 9.05	Introduction and purpose of the workshop	(F. Kautsky)
9.10 – 10.00	SKB presentations on selected topics specified in advance by SKI	
10.00 – 10.30	Coffee break	
10.30 – 12.00	SKB presentations on selected topics specified in advance by SKI	
12.00 – 13.00	Lunch	
13.00 – 15.00	Questions from working groups	(O. Stephansson/WG)
15.00 – 15.30	Coffee break	
15.30 – 16.30	Questioning cont'd	
16.30 – 17.00	Summation of workshop discussions	(O. Stephansson/WG)
18.00 – 19.00	***Invited lecture*** *(conference room Jensen Carlén)* Long-term characteristics of the clay barrier, assumptions and knowledge	(R. Pusch)
19.00	Dinner	

Wednesday, November 17th

(Conference room Sten Broman salen)

9.00 – 10.00	Discussion of outcome from questioning of SKB	(OS/WG chairs)
10.00 – 10.30	Coffee break	
10.30 – 12.00	Discussion and conclusions on implications for SKI work	(led by B. Strömberg)
12.00	End of meeting	
12.00	Lunch	
13. 00 - 17.00	Visit to the factory for fabrication of bentonite blocks in Ystad	(bus)
	The bus will stop at Sturup airport (c. 16.30) with a final stop at the Main Train Station in Lund (c.17.00) on its way back.	

List of participants

Eduardo Alonso	UPC, Spain
Mick Apted	Monitor Scientific, US
Randy Arthur	Monitor Scientific, US
Adrian Bath	IntelliSci, UK
Johan Claesson	CTH, Sweden
Jussi Heinonen	STUK, Finland
Jing Lanru	KTH, Sweden
Jonny Rutquist	LBNL, US
David Savage	Quintessa, UK
Ove Stephansson	GFZ, Germany
Göran Sällfors	CTH, Sweden
Chin-Fu Tsang	LBNL, US
Anders Wiebert	SSI, Sweden

SKI staff:

Behnaz Aghili
Christina Lilja
Fritz Kautsky
Bo Strömberg
Benny Sundström
Öivind Toverud
Stig Wingefors

SKB staff and consultants will participate the second day (Tuesday, November 16) between 09.00-17.00

SKB staff:
Allan Hedin
Tommy Hedman
Patrik Sellin

SKB consultants:

Lennart Börgesson	ClayTech
Ola Karnland	ClayTech
Harald Hökmark	ClayTech

Appendix B: Questions to SKB

B-1 Questions developed before the workshop

Questions sent to SKB in advance for the EBS workshop in Lund. Questions should be addressed by SKB in the morning session, Tuesday November 16th.

1. Present basis and rationale of the buffer and backfill function indicators (Table 1 of SR-CAN interim report (TR-04-11), and the criteria they should fulfil according to data in Table 1-4, p.14 of SKB R-04-33. Do not consider issues related to radionuclide transport and defect canister.

2. Present the current state-of-knowledge concerning DEPONIT CA-N bentonite, Friedland clay and low- alkaline cement as new materials for a future KBS-3 repository.

3. The long-term evolution of buffer and backfill will be governed by chemical and physical processes. These may occur in such a way that function indicators would change as a function of time. In what way will SKB handle the following alternatives in SR-Can (modelling work, experimental basis, performance confirmation tests etc):
   A) changes in the temperature interval 80-110C (e.g. cementation, formation of gaps and cracks)
   B) increase in groundwater salinity
   C) other changes in groundwater chemistry (that may affect the stability of e.g. smectite phases)
   D) combinations of A, B, C

4. How will SKB handle the possibility of permafrost at repository depth? How would freezing and thawing during a glaciation cycle affect buffer and backfill performance?

5. How will SKB address the cases where bentonite may be lost (piping/erosion) in SR-Can (modelling, experimental basis, performance confirmation tests etc)?

6. Discuss buffer processes (thermal, mechanical, chemical or hydraulic) and present an overview of the effects of these processes relative to:
   - Non-uniform bentonite swelling
   - Finite swelling pressure
   - Resaturation time
   - Pore water composition

   Will extremely long resaturation times (several hundred to thousands of years) be acceptable in SR-Can? If this is the case, how will SKB justify this?

7. How will the possibility/probability of canister sinking be addressed?

BE AWARE LIST (Issues for SKB to be prepared to answer as they may be raised at the meeting (Hearing session). No formal presentations are required by SKB in advance

- Interaction between buffer, backfill and host rock.
- Processes in slots and gaps
- Present state of knowledge about T-H-M-C modelling of buffer and backfill performance in the Prototype Repository experiment at Äspö H.R.L.
- Statistical significance of the likely processes of long-term performance
- Bentonite and EDZ: design and effectiveness of sealing EDZ with bentonite
- Bentonite and cement interaction
- Relevance of ongoing work for KBS-3 H
- Review state of art of modelling methods, and plans for further development, if any.

B-2 Complentary questions developed during the first day of the workshop

Introductory comment

- in the context of the buffer and backfill, it would be helpful if SKB could identify what information (field and laboratory experiments and modelling) will be available during the different licensing stages.

Question 1

- what procedures have SKB used to select the particular function indicators and associated criteria?
  - what is the 'margin of comfort' for function indicators? e.g. has SKB carried out sensitivity analyses?
  - in those considerations, has SKB considered whether coupling of functions might necessitate a re-evaluation of specific criteria?
- is there any time dependence of function indicators (buffer and backfill), and how will this be addressed?
- how does the potential formation of an EDZ affect SKB's assignment of function indicators for the buffer and backfill?

Question 2

- use of MX-80 is supported by a large R&D database, so how much of that is transferable to alternative bentonites?
- what research is anticipated on the interaction of low-alkali cement with other EBS components?

Question 3

- how will the issue of groundwater salinity affect different designs of backfill?
- what are SKB's plans to bound potential piping?
- is there a model for backfill erosion in low salinity groundwater?
- what is the strategy for evaluating THMC coupled processes in PA (e.g. mechanical effects of cementation)?
- is there a 'trade-off' in backfill designs to be able to meet the backfill function indicator of compressibility and permeability? If this is the case, how will this be handled?
- has SKB considered the deleterious effects of surface storage of crushed rock before its re-introduction as backfill?
- what are the impacts of cyclical changes in salinity?

Question 4

- SKI will be interested to see further research and analysis to address freezing/thawing at repository depths.

Question 5

- what is the detailed mechanism for piping and what are the local groundwater inflow conditions that are likely to exacerbate it?
- how much dependence can SKB place on the results of one experiment with respect to the piping issue? i.e. the prototype repository experiment to be excavated in 10 years' time

Question 6

- if there are long re-saturation times, how will SKB deal with this and what are the research needs?
  - what are the underlying assumptions that are involved in extrapolating the models of buffer processes to long re-saturation times?
- has SKB considered what may happen if the buffer is saturated before backfill saturation?
- how will heterogeneous saturation in the different backfill designs impact upon subsequent compliance with functional indicators? Does SKB plan experiments or modelling to test this?
- has SKB considered processes that might give rise to separation of materials in the backfill over long periods of time?

Appendix C: Extended abstracts

- **Laboratory Experiments. Present Status, Lessons Learned, Relevance for Radwaste and Pending Issues**
  Eduardo Alonso

- **Geochemical Models of Bentonite-Water Interaction: An Overview of the State-of-the-Art**
  Randy Arthur, Mick Apted, Mike Stenhouse

- **Drying and Resaturation of the Bentonite Barrier - New Tools for Modeling and Analysis**
  Johan Claesson, Göran Sällfors

- **STUK's View on Buffer and Backfill Issues. Review of Posiva's RTD Programme TKS-2003**
  Jussi Heinonen

- **State-of-the-Art of Coupled Thermal-Hydrological-Mechanical Processes in the DECOVALEX Project. Lessons Learned and Important Issues**
  Jonny Rutqvist

- **The Effects of High Salinity Groundwater on the Performance of Clay Barriers**
  David Savage

- **EC Activities on Geological Disposal of Radioactive Wastes**
  Ove Stephansson

SKI Workshop
EBS. Long Term Stability Of Buffer And Backfill
Lund, November 2004

LABORATORY EXPERIMENTS. PRESENT STATUS, LESSONS LEARNED, RELEVANCE FOR RADWASTE AND PENDING ISSUES

Eduardo E. Alonso
Professor of Geotechnical Engineering. UPC. Barcelona (Spain)

1 INTRODUCTION

A review is made of recent experimental results concerning the THM behaviour of bentonite. Most of the data presented corresponds to the Febex bentonite, a material which has been tested over the last 10 years within the framework of the Febex project. The Febex bentonite contains moderately plastic Ca-Mg montmorillonite. Its properties will not be necessarily equal to Na-based bentonites, such as MX-80 or Kunigel. However, this Note will focus on general trends and fundamentals of behaviour, which are of wider significance. Experiments presented have been performed by two laboratories: the CIEMAT Laboratory (Madrid) and the Geotechnical Laboratory of the UPC (Barcelona).

An account of the available knowledge on THM behaviour of Febex bentonite will be rather extensive. Some selective criteria have to be adopted in order to keep this note within the established limits. The following topics are believed to summarise most of the recent advances in understanding:

- Long term hydraulic behaviour of bentonite
- Temperature effects on hydro-mechanical response
- Solute effects on hydro-mechanical response
- Mechanical behaviour
- Microstructure evolution
- Tests in medium-scale cells
-

2 LONG TERM HYDRAULIC BEHAVIOUR OF BENTONITE

Discrepancies between model predictions and fields records of the evolution of relative humidity during hydration of “in situ” and “mock-up” Febex tests has raised the important issue of the reliability of our current THM formulations to predict hydration times of the bentonite buffer. Several phenomena have been invoked to explain the discrepancies: Evolution of the microstructural fabric of the bentonite, existence of a threshold gradient in Darcy’s law and thermo-osmotic effects. An additional potential explanation is proposed here: the change in water density as the free water coming from the surrounding rock becomes the inter-lamellar water when the bentonite saturates.

Bentonite identification after conducting swelling pressure tests reveals that the calculated degree of saturation (for $\rho_w = 1$ g/cm^3) is systematically larger than one. Consistency is achieved if the water density in the adsorbed phase is larger than 1 g/cm^3. Available data (Fig. 1) indicates that the average water density for the void ratios reached in the Febex project may reach 1.15 g/cm^3. This is consistent with a density of 1.2 g/cm^3 for the adsorbed water. Theoretical results can also be involved to explain the increase in density of the adsorbed water layers within the inter-lamellar distance. The number of water layers in this space is controlled by the RH (suction) or, alternatively, by the confining stress. When the bentonite is saturated in the buffer, the swelling pressure provides the confinement stress to maintain a reduced number of water monolayers in the inter-lamellar space.

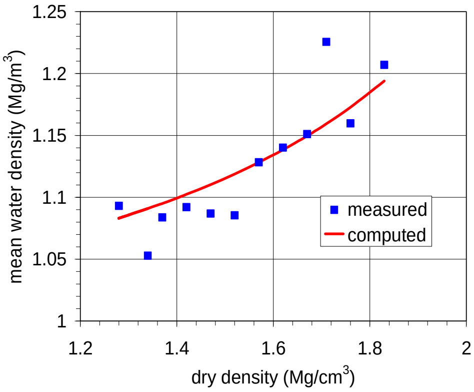


Figure 1: Apparent average water density calculated for saturated specimens at the end of swelling pressure tests

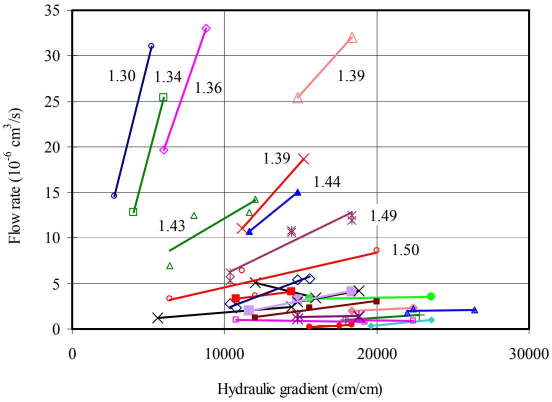


Figure 2: Long term hydraulic behaviour of bentonite. Threshold gradient (CIEMAT tests)

One of the implications of the increased density is that increased volumes of free water ($\rho_w = 1$ g/cm^3) are required to saturate the buffer. The phenomena may be modelled as a phase change affecting the infiltration water.

Tests to investigate the existence of a threshold gradient have not been conclusive so far. Figure 2 shows the relationship between flow rate and hydraulic gradient for compacted bentonite specimens of varying density. The straight segments plotted seem to pass through the origin. Note, however, that the minimum gradients applied are in the order of a few thousands. Tests imposing smaller gradients are required.

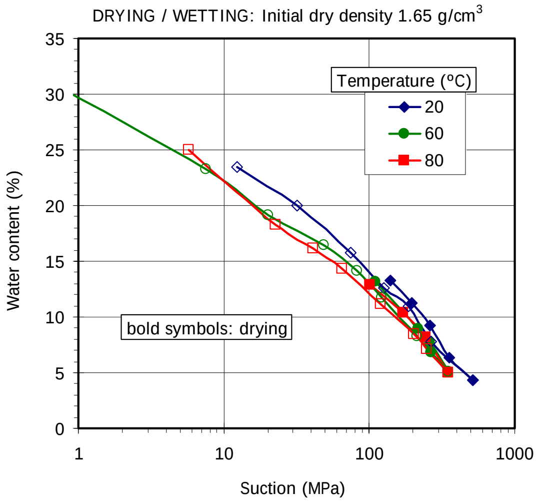
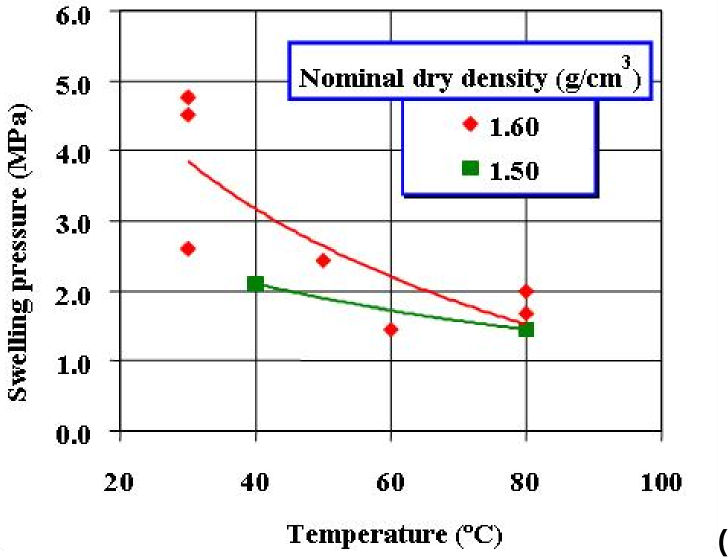


Figure 3: Temperature effects on water retention curve of Febex compacted bentonite.

3 TEMPERATURE EFFECTS ON HYDRO-MECHANICAL RESPONSE

Temperature within the range 20-80 ºC seems to have a limited effect on hydraulic properties of compacted bentonite. Some results are shown in Figure 3 for the water retention curve. No systematic effect of temperature on swelling under load tests has been obtained. However, the swelling pressure seems to be more sensitive to temperature changes (Fig. 4). Apparently the swelling pressure decreases with increasing temperature. A swelling pressure of no more than 1 MPa is found for the Febex bentonite at $\gamma_d = 1.6$ g/cm^3, when T = 100 ºC.



(a)

Figure 4: Swelling pressure tests performed in temperature controlled oedometer cells.

Temperature effects on clays (both saturated and unsaturated) has been reported in a relatively large list of publications over the past decade. Most of the experimental observations are consistent with a decrease of yield mean stress as the temperature increases. This is also consistent with the reported decrease in swelling pressure as temperature increases.

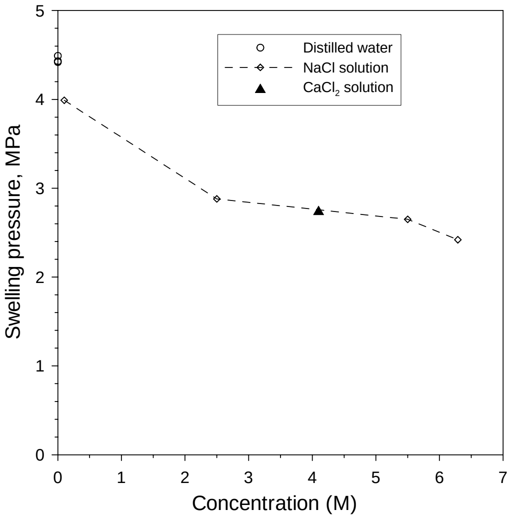


Figure 5: Swelling pressure values for different concentrations and solutions,(γd =1.65 g/cm3).

4 SOLUTE EFFECTS ON HYDRO-MECHANICAL RESPONSE

The salt content of the free water added to saturate the compacted bentonite has a noticeable effect on measured hydraulic conductivity and on swelling behaviour. Figure 5 shows, for instance, the decease in swelling pressure as the salt concentration of the added water increases. However, in order to obtain these effects the salt concentration has to increase substantially. Measured salt concentration in the water, extracted from specimens taken from the Febex bentonite ring after dismantling, show minor concentrations of salt (in the order of 2-6 x 10^{-4} M), which, in view of Figure 5, implies a negligible effect. Environments with higher salt concentrations may lead to a different conclusion.

5 MECHANICAL BEHAVIOUR

Available data on stress distributions of large scale tests provide an idea of the stress paths followed by different points of the bentonite buffer. In particular, it is interesting to know if significant shear stresses may be induced. Data from the analysis of the Febex mock-up test (Fig. 6) show that the stress paths in a (q, p) plane do not reach limiting conditions. There is, however, a significant lack of information concerning the deviatoric behaviour of compacted bentonite. Under confined conditions (this is the case of the tunnels in granite) the bentonite follows a “swelling pressure” type of path (increase in average stress as the suction decreases). Some designs, however, (existence of a sand layer at the buffer-rock contact) may lead to significant deviatoric stress development.

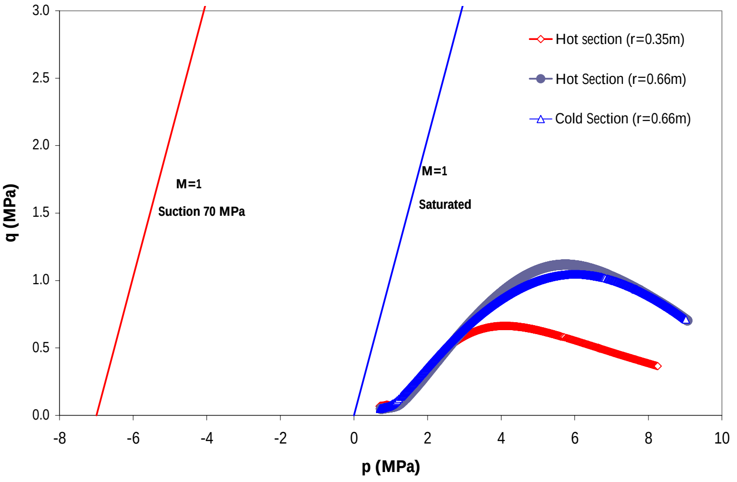


Figure 6: Mechanical behaviour. Stress paths in Febex Mock-up test

Suction controlled testing of bentonite behaviour under oedometric conditions is generally available. A simple interpretation of these tests, through a "state surface" approach provides a simplified volumetric constitutive behaviour. A more fundamental elasto-plastic approach may be used to describe the mechanical behaviour of bentonite. A key information for these models is to establish the variation of (average) yield stress with suction. Suction controlled swelling pressure tests provide a good approximation to the effect of suction on yield stress, as shown in Figure 7. The figure shows a significant increase of yield stress with suction.

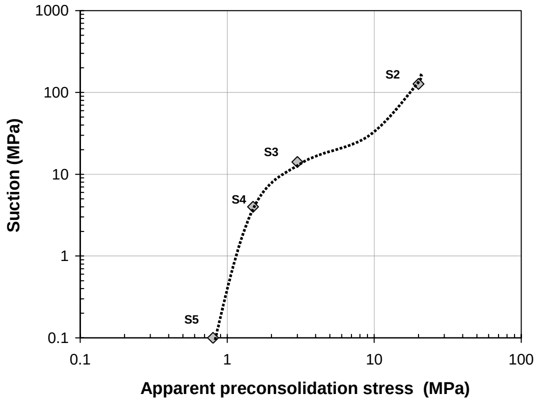


Figure 7: Apparent yield stress of compacted febex bentonite as a function of suction

6 EVOLUTION OF MICROSTRUCTURE

Advanced THM modelling requires a knowledge of the evolution of the internal structure of the bentonite. In fact, changes in pore distributions lead to major changes in the intrinsic permeability. On the other hand, swelling of the basic structural units explains the overall macroscopic behaviour. A useful information on the evolution of microstructure is provided by the evolution of pore size distribution. It has been found that, upon wetting, the relatively large pores existing at the time of compaction tend to disappear and to transform into lower pore sizes (two orders of magnitude smaller).

Some elastoplastic models describe the mechanical behaviour of the bentonite, in terms of two interacting continua: one represents the expanding/shrinking basic microstructural units, and the other accounts for the large porosity between clay aggregates. These models deal to a more accurate representation of the measured response of specimens under suction-controlled testing.

7 TESTS IN MEDIUM SCALE CELLS

Improved capabilities for fully coupled THM backanalysis using finite elements programs have provided a powerful interpretation of tests run in cells so that the usual requisite of uniform stress/strain or hydraulic gradient is no longer enforced. Rather the idea is to conduct tests, which reproduce, to some extent, the conditions existing in situ. They are, in fact, boundary value problems. If data on different variables is measured (relative humidity, temperature, stresses) backanalysis procedures may be used to derive material parameters. Some of the parameters that could be derived in this way are not easy to measure under conventional testing, for instance, the unsaturated hydraulic conductivity on the tortuosity factor. One example is the thermo-hydraulic cell developed at UPC in which a temperature gradient was imposed on a symmetric arrangement of cylindrical specimens of compacted bentonite. Temperature was measured at selected points and, once the test was finished, the water content distribution along the two specimens was determined. The interpretation (Figure 8) provides estimates of the relative permeability and the tortuosity factor.

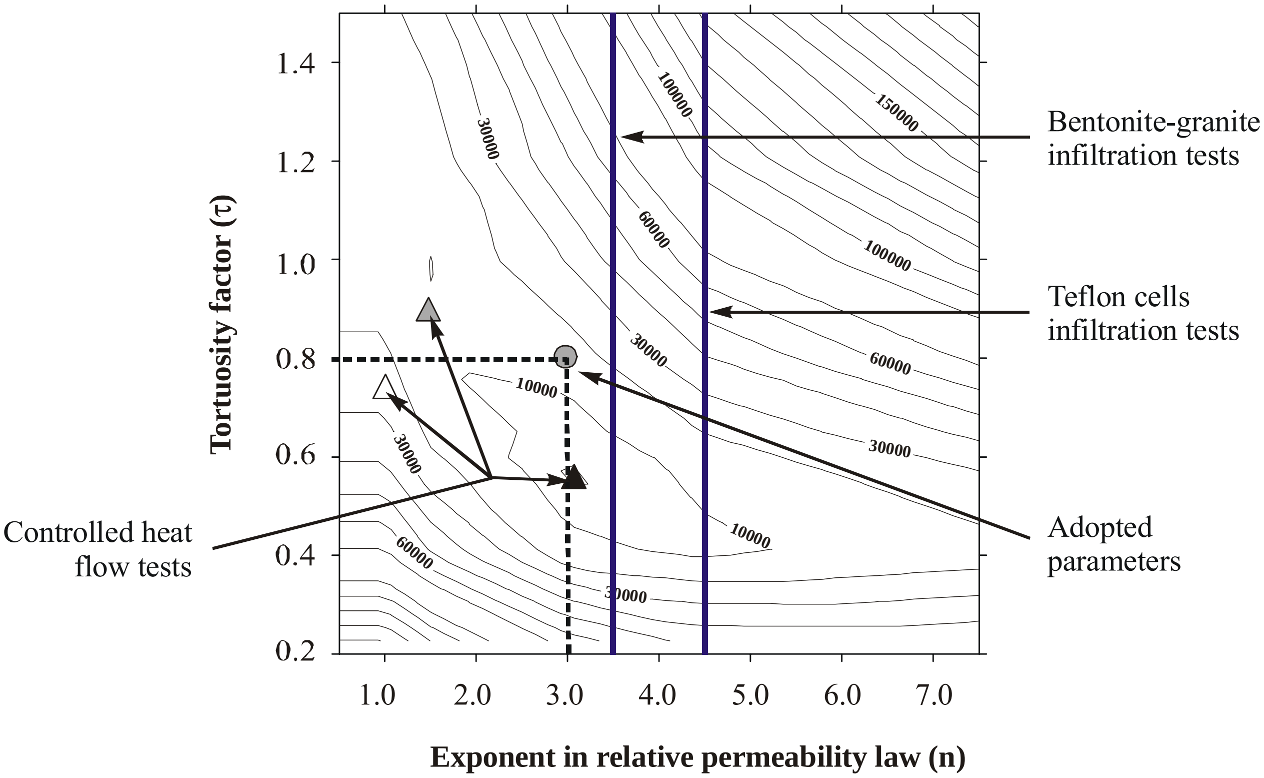


Figure 8: Contour map of objective function.

8 CONCLUSIONS

The following conclusions can be established:

- Long term hydraulic behaviour
    - Water hydrating the buffer, under pressure, seems to increase its density. It is interpreted as a phase change phenomena, which may lead to increased times for buffer hydration
    - There is no experimental evidence so far of a threshold effect concerning he Darcy's law.
- Temperature effects
    - Minor temperature effects on hydraulic behaviour has been detected in the range 20 ºC -80 ºC
    - A significant reduction of swelling pressure with temperature has been measured
    - Temperature seems to reduce the apparent yield locus of clays
- Solute effects
    - Noticeable solute effects on hydraulic and mechanical properties are found for very large changes of solute concentration (>1M)
    - Measurements after dismantling Febex show very small changes in solute concentration
- Mechanical behaviour
    - Stress paths in confined buffers reproduce "swelling pressure" type of paths. Deviatoric components are of less significance, but there is a lack of experimental data on the deviatoric behaviour of compacted bentonite
    - In arrangements which imply a loss of confinement, significant deviatoric stresses may develop
    - Suction controlled testing allows a comprehensive constitutive mechanical characterization of the compacted bentonite
- Evolution of microstructure
    - Major changes in porosity distribution are associated to bentonite hydration. They can be followed using MIP techniques and they provide a good understanding of the evolutionary character of an expanding buffer
    - Double porosity models provide increased modelling capabilities
- Tests in medium scale cells
    - Back analysis techniques using fully coupled THM codes are a powerful procedure to derive material parameters
    - Medium scale cells complement successfully standard testing on small homogeneous samples

Geochemical models of bentonite-water interaction: An overview of the state of the art

Randy Arthur, Mick Apted and Mike Stenhouse
Monitor Scientific, LLC
Denver, Colorado USA

INTRODUCTION

This paper provides a brief overview of models that could be used to assess the long-term chemical evolution and mineralogical stability of bentonite buffer and backfill materials in a KBS-3 repository. Models currently favored by SKB are of special interest. The objective in preparing this paper is to help provide a starting point for discussions to be held at an upcoming SKI workshop on the same subject. The results of the workshop will be used to formulate SKI's views on uncertainties and the significance of various processes that could occur within the buffer and backfill. These views will provide a foundation for regulatory review of SKB's future license applications for the encapsulation plant and deep repository.

CHEMISTRY OF THE SMECTITE CLAYS

A complicating factor in models of buffer and backfill stability is the fact that the chemistry of the smectite clays, which are the dominant mineral constituents of these bentonite-containing barriers, is variable within limits (*e.g.,* Velde, 1992). Three groups of dioctahedral smectites[1] are classified based on their Al and Fe^{3+} contents. Aluminous varieties include the beidellites and montmorillonites. Nontronites contain relatively high concentrations of Fe^{3+}. There is a complete solid-solution compositional range between the nontronites and beidellites, and a significant, but incomplete, compositional range between the montmorillonites and beidellites. Trioctahedral smectites, which are also swelling clays, include saponites and stevensites. Saponites are aluminous whereas stevensites are essentially devoid of Al.

The variable chemistry of smectites can be related to their crystalline structure. These clay minerals have a 2:1 lattice structure consisting of one octahedrally coordinated layer between two tetrahedrally coordinated sheets. Ionic substitutions in the octahedral and tetrahedral layers result in a net negative charge on the 2:1 framework, which is compensated by hydrated cations occupying interlayer positions. Interlayer charge originates from ionic substitutions in the tetrahedral layer of beidellites (mainly Al^{3+} for Si^{4+}), and from ionic substitutions in the octahedral layer of montmorillonites and nontronites (divalent cations for Al^{3+} in montmorillonites and divalent cations, including Fe^{2+}, for Fe^{3+} in nontronites). Interlayer charge in dioctahedral smectites can vary widely between roughly 0.2 to 0.6 equivalents per 2:1 unit of $O_{10}(OH)_2$ anionic charge. These minerals may thus be stable over a considerable range of environmental

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[1] The term dioctahedral indicates that two thirds of cation sites in the octahedral layer of the clay's crystalline lattice (see below) are occupied; all of these sites are occupied in trioctahedral smectites.

conditions and associated ranges in porewater chemistry. Cations occupying the interlayer sites typically include Na^+, Ca^{2+}, Mg^{2+} and K^+.

MODELS OF BENTONITE-WATER INTERACTION

A number of models have been proposed for simulating the long-term chemical and mineralogical evolution of buffer and backfill materials. Most of the models assume equilibrium. They differ according to the types of reactions considered for the clay minerals. From simplified to comprehensive, the models account for fixed-stoichiometric, ion-exchange, surface-chemical and isomorphous-substitution reactions. Kinetic models have also been proposed for the alteration of smectite to illite. The equilibrium and kinetic models are described below.

Stoichiometric models. These models are based on the assumption that smectites have a fixed stoichiometric composition (*e.g.,* Garrels, 1984). This assumption, although clearly unrealistic for smectites in general (as discussed in the preceding section), allows conventional activity-activity diagrams to be used to evaluate the thermodynamic stability of a *representative* smectite composition relative to other clay and non-clay minerals. The models can thus be used to establish approximate stability boundaries among the various dioctahedral and trioctahedral smectites, as well as between smectites and other minerals. This approach has not been used extensively by SKB (see, however, Tardy *et al.*, 1987).

Ion-exchange models. Ion-exchange reactions involve rapid displacement of interlayer cations and replacement with cations in a coexisting aqueous phase (*e.g.,* Garrels and Christ, 1965). This process is assumed to occur without an appreciable compositional change in the basic 2:1 structural unit of the clay. Because the composition of this unit is fixed, it does not have to be treated explicitly with respect to mass-balance and charge-balance constraints imposed by a balanced chemical reaction.

Ion-exchange reactions considered by SKB for bentonite buffer materials include replacement of Na^+ in montmorillonite by Ca^{2+} or Mg^{2+} (Wanner *et al.,* 1992; Bruno *et al.,* 1999)[2]. The reactions are represented by:

$2NaX + Ca^{2+} = CaX_2 + 2Na^+$; and

$2NaX + Mg^{2+} = MgX_2 + 2Na^+$,

where X refers to the clay's 2:1 structural unit, or "layer surface site" (Wanner *et al.,* 1992). The equilibrium constant, K, for the first reaction (for example) is given by:

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[2] Wieland *et al.* (1994) propose similar reactions involving exchange of Na^+ by H^+ at interlayer sites on the "external surfaces" of montmorillonite (so-called "X" sites) as well as on "internal surfaces" of a montmorillonite "platelet" ("Y" sites). These reactions are not considered in further refinements of SKB's model (Bruno *et al.* 1999) because they are unimportant relative to other surface reactions involving H^+ (see below).

$$K = K_c \frac{\gamma_{Na^+}^2}{\gamma_{Ca^{2+}}}, \qquad (1)$$

where γ refers to an activity coefficient for the free aqueous species and K_c stands for a conditional equilibrium constant. The conditional constant is valid only for a specific surface composition, ionic strength and temperature, and is given by:

$$K_c = \frac{[\mathrm{Ca}X_2][\mathrm{Na}^+]^2}{[\mathrm{Na}X]^2[\mathrm{Ca}^{2+}]},$$

where the brackets denote concentration per unit volume of the aqueous solution. Equation (1) is derived assuming that activity coefficients for the sorbed cations equal unity. This may be a valid assumption, based on limited experimental data (see Wanner *et al.*, 1992), provided changes in the concentrations of the surface species are not too large.

Wanner *et al.* (1992) used unpublished experimental data from SKB on the interaction of untreated MX-80 bentonite with distilled water or synthetic Swedish-type granite groundwater ("Allard water") at room temperature to estimate values of log K for the Na-Ca and Na-Mg exchange reactions[3]. Interpretation of these experimental results is not straightforward because dissolution of accessory minerals in the bentonite may have affected the aqueous concentrations of some important cations (notably Ca^{2+}) and anions (SO_4^{2-}), and because it is unclear whether equilibrium was attained for all relevant reactions, including the exchange reactions. The log K values estimated by Wanner *et al.* (1992) are nevertheless reasonably similar to those determined by Olin *et al.* (1995). The latter study retrieved exchange constants from experimental data obtained over a period of up to 9 months at 75°C in a system consisting of copper cylinders packed with MX-80 bentonite and reacted with Allard water or Allard water containing a 100-fold increase in K^+. The fair agreement between the exchange constants determined by Wanner *et al.* (1992) and Olin *et al.* (1995) is somewhat surprising given the significant differences in experiment design and experimental conditions considered in these two studies.

Surface-complexation models. In addition to the charge resulting from ionic substitutions within the crystalline lattice of smectite, ionization of surface OH groups can also generate a variable, pH-dependent charge. Deprotonated OH groups form surface complexes with metal ions, and thus have a minor influence on the overall composition of these clay minerals. More importantly, such surface-complexation reactions control the colloidal stability of smectites, as well as their sorption behavior with respect to trace concentrations of transition metals, actinides and fission products. Like ion-exchange models, surface-complexation models do not account explicitly for the composition of smectite's 2:1 layer framework.

The following reactions are considered in SKB's surface-complexation model for the buffer (Wieland *et al.*, 1994):

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[3] The Na-K exchange reaction cannot be evaluated from these data because K^+ was not measured.

$\equiv SOH_2^+ = \equiv SOH + H^+$, and

$\equiv SOH = \equiv SO^- + H^+$

where $\equiv SOH_2^+$, $\equiv SOH$ and $\equiv SO^-$ represent positively charged, neutral and negatively charged surface hydroxyl groups, all of which are assumed to exist at edge faces of individual montmorillonite crystals. The corresponding mass-action expressions are given by:

$$K_{a1}^{\text{int}} = \frac{(\equiv \text{SOH})(\text{H}^+)}{(\equiv \text{SOH}_2^+)} \exp(-\frac{F\Psi}{RT}), \text{and}$$

$$K_{a2}^{\text{int}} = \frac{(\equiv \text{SO}^-)(\text{H}^+)}{(\equiv \text{SOH})} \exp(-\frac{F\Psi}{RT})$$

where K_{a1}^{int} and K_{a2}^{int} represent intrinsic acidity constants, ( ) denotes activity of the indicated surface species, or of H^+ in the bulk solution, Ψ stands for the electrical potential at the clay surface, and F, R and T refer to the Faraday constant, gas constant and temperature, respectively. Bruno *et al.* (1999) ignore contributions to K_{a1}^{int} and K_{a2}^{int} arising from electrostatic potentials near the clay surface, and thus effectively assume $\Psi = 0$ in the above equations.

Wieland *et al.* (1994) carried out acidimetric and alkalimetric titrations of Na-montmorillonite suspensions at room temperature. The starting montmorillonite was purified from MX-80 bentonite. Parameters in a model accounting for the surface complexation reactions discussed above were fit to the measured titration curves. Retrieved values at ≈ 25°C include $\log K_{a1}^{\text{int}} = -5.4 \pm 0.1$ and $\log K_{a2}^{\text{int}} = -6.7 \pm 0.1$. The total number of surface-complexation sites = 2.8×10^{-5} mol g^{-1}. Bruno *et al.* (1999) state that the titration data of Wieland *et al.* (1994) are the only experimental data available for smectites.

Isomorphous-substitution reactions (solid-solution models). These reactions include ion-exchange reactions as well as substitution of cations in octahedral and tetrahedral coordination within smectite's 2:1 lattice structure. Solid-solution models treat these reactions in terms of changes in the activities of thermodynamic components. Two solid-solution models have been proposed for smectites. They differ depending on whether component activities are assumed to be controlled by ideal mixing of end-member components or by ideal site-mixing of individual atoms occupying the clay's interlayer, octahedral and tetrahedral sites. SKB sponsored early work on ideal-mixing models for smectite (Fritz and Kam, 1985; Tardy *et al.*, 1987), but this work now appears to have been discontinued. Cramer and Smellie (1994) used an ideal site-mixing model to interpret the chemistry of porewaters in argillaceous rocks of the Cigar Lake natural analogue site. A limitation in applying solid-solution models to clay minerals is that the thermodynamic properties of the components are not generally well known and may have to be estimated.

Illitization models. The stability of the smectite clays is often considered in terms of reactions involving the transformation of smectite to illite. These reactions have been studied in considerable detail by SKB and others. Karnland *et al.* (1995) provide a useful review of these studies.

The mechanism by which montmorillonite is transformed into illite is not well understood, but the overall process can be represented in terms of the following schematic reaction:

$$\text{montmorillonite} + Al^{3+} + K^{+} \rightarrow \text{illite} + Si^{4+} + Ca^{2+}/Na^{+} + Fe^{2+}/Mg^{2+},$$

where the right-facing arrow emphasizes the possibility that the transformation rate is extremely slow. Whether the reaction involves a solid-state, layer-by-layer replacement of smectite by illite, or complete dissolution of smectite followed by precipitation of neoformed illite, is still an open question. In general, however, the reaction results in an increase in layer charge due to replacement of Si^{4+} by Al^{3+} at tetrahedral positions, a decrease in the Fe^{2+} and Mg^{2+} content of octahedral sites and an increase in interlayer K^{+} at the expense of other interlayer cations, including Na^{+} and Ca^{2+}.

The rate of smectite alteration can be modeled using a kinetic expression such as (Huang *et al.*, 1993):

$$-\frac{dS}{dt} = A\exp\left(\frac{-E_a}{RT}\right)(\mathrm{K}^{+})S^{2},$$

where S stands for the fraction of smectite relative to smectite + illite, t represents time in seconds, A denotes a frequency factor (= $8.08\text{x}10^{4}$ liter mol^{-1} sec^{-1}), E_a refers to an activation energy (= 28 kcal mol^{-1}), (K^{+}) indicates molar concentration, and R and T stand for the gas constant and temperature (°K), respectively. Karnland *et al.* (1995) use this model with reasonable K^{+} concentrations in typical granite groundwaters and expected temperatures in the KBS-3 near field to show that almost all of the smectite in the buffer and backfill would not be converted to illite even after 1 million years of repository evolution. These authors also point out, however, that the model considers changes only in K^{+} concentration, whereas other cations are known to be involved in the transformation reaction and may have an accelerating or inhibiting effect on the reaction rate, and that there is some uncertainty in the Arrhenius parameters A and E_a, which could affect the calculated reaction rate.

COMMENTS ON SKB'S MODEL OF BUFFER AND BACKFILL STABILITY

The following comments are based on the assumption that long-term mineralogical changes in the buffer (and backfill) could have an adverse impact on the assigned isolation functions and properties of these barriers (*e.g.,* see SKB, 2004). This assumption is consistent with qualitative and quantitative observations relating such properties and functions to the mineralogy of bentonite (*e.g.,* Pusch, 1996).

SKB's current model of the chemical and mineralogical evolution of the KBS-3 buffer is described by Domènech *et al.* (2004) and SKB (2004). The chemical composition of smectite (*i.e.,* montmorillonite) is not considered explicitly in the model. Rather ion-exchange and surface-complexation reactions involving this mineral are modeled using the approaches described by Bruno *et al.* (1999), Wieland *et al.* (1994) and Wanner *et al.* (1992). Transformation of smectite to less-expandable minerals is modeled using a kinetic expression and a transport model for dissolved silica.

SKB's ion-exchange and surface-complexation models refer to a specific, though unspecified, composition of the clay's negatively charged 2:1 framework. To apply such models it must be assumed that this lattice composition does not change over the time period of interest (Garrels and Christ, 1965). This assumption may be unrealistic, however, given the 100,000 year lifetimes now being considered for intact canisters. Although little is known about how quickly smectite's lattice chemistry can change as a result of ionic substitutions on all of its structural and exchange sites, the widely variable compositions of these minerals in natural systems suggests that it is possible that significant changes in mineral chemistry, possibly including complete conversion of the initial montmorillonites to beidellites, saponites, *etc.*, could occur within 100,000 years. The absence of, and difficulty in collecting, such information is not a valid reason for excluding the possibility that such reactions may occur and potentially modify the isolation capabilities of the buffer. SKB is therefore encouraged to defend and document its approach as (1) comprehensive, realistic and testable, or (2) credibly bounding with respect to providing assurance that isolation functions and properties of the buffer will be maintained over repository-relevant time scales. Any plans by SKB to evaluate and implement additional models accounting for long-term substitution reactions in smectites should also be identified.

SKB's approach is not based on the thermodynamic behavior of the smectite clays. Rather, it simply assumes that the montmorillonite initially present in the buffer and backfill is stable indefinitely, or, if not, that it slowly alters to a less expandable mineral at a predictable rate. This simplifying assumption may not be acceptable from a regulatory point of view because it obviates the need for understanding the specific conditions of clay-mineral stability/instability in relation to evolving geochemical environments in the near field and far field, and because it may overemphasize the importance of accessory minerals and surface reactions in controlling the long-term chemical evolution of these barriers.

Dissolution, transport and precipitation processes during the resaturation phase and transient thermal period of repository evolution could cause individual clay particles in the buffer to become cemented together, thereby possibly adversely affecting the desirable physical and rheological properties of this barrier. SKB plan to ignore the resaturation phase and to consider reactions involving only a few "impurity" minerals during the thermal period (*e.g.,* Arcos *et al.,* 2000). Ignoring the dominant clay minerals in the buffer as potential sources of cement-forming elements like Si and Al may cause such simplified models to seriously underestimate the extent of cementation.

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DRYING AND RESATURATION OF THE BENTONITE BARRIER. NEW TOOLS FOR MODELING AND ANALYSIS.

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1. Heat and moisture flow problem

The bentonite, which surrounds and protects the canisters in a nuclear waste repository deep down in rock, experiences a complex coupled heat and moisture flow process. The emitted heat from the canisters will cause an initial drying from the warmer canister side. The water in cracks and fractures in the rock will on the other hand cause successive saturation of the bentonite from the outer rock side. These processes will interact and a key question is the degree of initial drying and the time it takes to saturate the bentonite under various scenarios. Too much drying of the bentonite may damage its swelling and sealing capacity. The worst case with the strongest drying will occur for a canister in completely dry rock without any water supply from the adjacent rock.

The goals of this study are: (1) find methods to quantify the drying and resaturation, (2) study parameter sensitivity and identify key parameters, and (3) provide independent methods to test other numerical models. These coupled heat and mass processes have been studied with large numerical codes. This is a complementary study with a focus on *understanding* and with an endeavor to provide *handy models*.

This extended abstract presents results from Claesson (2004) and from Claesson, Hagentoft and Sällfors (2003).

2. Outline of the study and the analyses

The largest drying occurs in the center of the repository with the highest temperatures. We consider in particular the central canister. The drying is driven by water vapor diffusion. The highest drying occurs for the largest temperature gradient in the bentonite around the canister. This largest gradient from the warm canister will occur at the mid level of the canister, since heat may “escape” more easily from top and bottom of the canister. At the mid level of the canister, the heat and moisture flow process in the bentonite annulus is radial without any vertical component. We have only to consider *a radial, one-dimensional process* in the bentonite. This is an important simplification.

The first step in the analysis is to determine the temperature distribution over the bentonite annulus $(r_c < r < r_r,\ z = 0)$ as function of time. The temperature depends on the heat release $Q_c(t)$ from the central canister and from neighboring canisters. More and more canisters must be accounted for as time goes. The heat release decays exponentially with a time scale of some thirty years. The time scale to approach steady-state temperature conditions over the bentonite annulus is below 24 hours. This means that the temperature distribution over the annulus is virtually a steady-state one with a slow change on a time scale of years. A remarkably simple explicit formula for the temperature $T_{\mathrm{r}}(t)$ in the bentonite at the rock boundary $(r = r_{\mathrm{r}})$ is presented in next section. The quasi steady-state temperature distribution in the bentonite is determined by $T_{\mathrm{r}}(t)$ and $Q_{\mathrm{c}}(t)$. The thermal process is essentially *decoupled* from the moisture flow process.

The equations for moisture flow in the bentonite annulus are discussed in Section 3. The total moisture flux has a liquid and a vapor component. The description of the flow involves data and functions for water and bentonite, and in particular for liquid and vapor flow in the bentonite. The moisture flux is determined by gradients in moisture state variables and temperature. We will choose the degree of water saturation in the bentonite *S*, $0 \le S \le 1$, as our basic moisture state variable. The flow coefficients before the gradients in *S* and *T* become functions of *S* and *T*.

We will restrict this study to the moisture flow in the bentonite annulus. The inner boundary against the canister is certainly watertight with zero moisture flux at $r = r_{\mathrm{c}}$. At the outer boundary $r = r_{\mathrm{r}}$, there are two limits. The rock may be sufficiently wet to maintain full saturation at the surface of the bentonite: $S_{\mathrm{r}} = 1$. We will call this the *wet-rock case*. The other limit, which is the worst possible case, is that the water flow to the rock is zero: $G_{\mathrm{r}} = 0$. We will call this the *dry-rock case*. (The possibility that the rock sucks water from the bentonite is ruled out, since the suction pressures are so high in bentonite.) The case with high water pressure at the outer bentonite boundary from a water table well above the repository is not discussed here, since it is a more favorable case, which will occur after a longer period of water recovery on repository scale.

With the reference data (3.6), we will find that the time scale to approach (exponentially) steady-state moisture conditions is around 4 years in the wet-rock case, and around 1 year in the dry-rock case. The temperature and the heat release from the canisters have, except for the first few years, a distinctly longer time scale. This means that the *steady-state* solutions for the moisture distribution over the bentonite annulus are quite interesting to us.

The steady-state solutions for the moisture distribution are studied in Section 4. One model deals with the general solution for $S(r)$ and $T(r)$ from two coupled, highly nonlinear, ordinary differential equations. From the structure of the coupled differential equations we find that there is an intrinsic relation between *S* and *T* that is *independent* of the radius *r*. We get a set of curves for $S = S(T; S_{\mathrm{r}})$ for different degree of water saturation S_{r} at the rock boundary $r = r_{\mathrm{r}}$. These diagrams give directly the drying and moisture distribution over the bentonite annulus in steady state for any moisture level and any temperature interval over the bentonite. A program for this generates a new diagram for any particular set of assumptions and data in a few seconds.

The time-dependent moisture process in the bentonite is studied in Section 5. The basic equation for $S(r,t)$ has a convective-diffusive character with a diffusivity function $D(S,T)$ and a convective-diffusive or thermo-diffusive coefficient function $A(S,T)$. The model that calculates these functions for any particular set of assumptions and data shows that the variations of these functions are rather moderate. In a process within a temperature span of 10°C and a degree of saturation from 0.75 to 1, the two coefficient functions vary some 20%. We may use *constant mean values* with an error below 10%.

These constant mean values depend on the saturation and temperature levels in the bentonite for the considered process. We have two basic parameters: the *mean diffusivity* D_0 ($\mathrm{m^2/s}$) for moisture flow and a dimensionless *thermo-diffusive parameter a*. The diffusivity determines the time scale to obtain steady-state conditions. The time scale is inversely proportional to the diffusivity. The second basic parameter *a* depends of the ratio between vapor and liquid diffusion coefficients. It is also proportional to the heat flux $Q_c(t)$. It increases with the temperature level.

We have in this approximation obtained a *linear* partial differential equation for $S(r,t)$. The general solutions of this equation have been derived for the dry-rock and wet-rock cases. From these solutions, explicit expressions for the maximum drying at the canister and the subsequent resaturation in the wet-rock case are derived. From these solutions, we have formulas and diagrams that give the complete transient process for any parameter values and initial degree of saturation: D_0 or a, t_0 and S_{in}. The two solutions have been implemented in Mathcad.

The linear approximation may also be used as a quite good approximation for the steady-state moisture profiles. In steady state, full saturation $S=1$ prevails through the bentonite annulus in the wet-rock case. In steady state for the dry-rock case, we get, in the linear approximation, a neat *explicit formula* for the degree of saturation as function of the radius (4.11). *The only parameters* are a and S_{in} (and the ratio of radii r_c / r_r). The *largest possible drying* in the bentonite occurs in steady state at the canister boundary for the dry-rock case. We get a single, very handy formula, (4.12), and diagram for the largest possible drying under any circumstances with a and S_{in} as parameters.

The key factors that determine the drying are discussed in Section 6. We may formulate two rules of thumb that the influence from the more important parameters.

Section 7 gives a survey of the new models and tools of analysis. All models involve a number of explicit formulas. They have been implements in Mathcad. It should be straightforward to implement the formulas in any other program such as Matlab or Maple.

Any calculation with the models require a few seconds only, except for the full solution of the linearized equations for $S(r,t)$, which may require a few minutes to determine the complete transient moisture flow process.

All models may easily be changed for other assumptions about flow coefficients, data, etc.

3 Equations

3.1 Flow equations

The moisture flux per unit area, g (kg/(m^{2}s)), in the bentonite has a liquid and a vapor component. The liquid flux g_{liq} is proportional to the gradient of the pore water pressure P with a hydraulic conductivity $k(S)$ that is a function of the degree of water saturation S. The flux is inversely proportional to the temperature-dependent viscosity $\eta(T)$. The water vapor flux g_{vap} is proportional to the gradient of the water vapor density ρ_v in the gas phases in the pores with a vapor conductivity factor $D_v(S)$ that is a decreasing function of S. We have:

$$g = g_{liq} + g_{vap}, \qquad g_{liq} = -\frac{\rho_w k(S)}{\eta(T)} \cdot \frac{\partial P}{\partial r}, \qquad g_{vap} = -D_v(S) \cdot \frac{\partial \rho_v}{\partial r}. \tag{3.1}$$

The heat or energy flux q (W/m^2) has a conductive part with a thermal conductivity $\lambda(S)$, which is a function of S. The convective part is equal to the liquid and vapor fluxes multiplied by their respective heat contents (specific enthalpy). We have

$$q = -\lambda(S) \cdot \frac{\partial T}{\partial r} + h_{liq}(T) g_{liq} + h_{vap}(T) g_{vap}. \tag{3.2}$$

We will see that the convective parts may be neglected.

We consider the total radial flux over the canister height H_c. The area of the cylinder at a radius r is $2\pi r H_\mathrm{c}$. The total fluxes of heat, Q (W), and moisture, G (kg/s), become

$$Q(r,t) = 2\pi r H_\mathrm{c} \cdot q(r,t), \qquad G(r,t) = 2\pi r H_\mathrm{c} \cdot g(r,t). \tag{3.3}$$

3.2 Data for bentonite and water

We will use the degree of water saturation S in the pores and the temperature T as basic state variables. The degree of saturation lies in the interval $0 < S \le 1$.

The water retention curve $P(S)$ is an important material property. We use the following functions for the bentonite

$$k(S), \quad D_\mathrm{v}(S) = D_\mathrm{v}(0) \cdot (1-S), \quad \lambda(S), \quad P(S). \tag{3.4}$$

The vapor diffusion coefficient $D_\mathrm{v}(S)$ is zero for $S = 1$, and it is proportional to $1-S$ in a first approximation

We also need data for water. We will use the saturation water vapor density, the water vapor density as a function of S and T, the dynamic viscosity, the heat of evaporation, and the heat content of water in liquid and vapor form:

$$\rho_\mathrm{v,sat}(T), \qquad \rho_\mathrm{v}(S,T), \qquad \eta(T), \qquad L_\mathrm{evap}(T), \qquad h_\mathrm{liq}(T), \qquad h_\mathrm{vap}(T). \tag{3.5}$$

All above functions for bentonite and water are represented by explicit formulas with an error below 1% in the interval $10 < T < 100$ °C and $0.3 < S \le 1$. The mathematical program Mathcad is used. All the functions (3.4) and (3.5) are discussed further in Claesson, Hagentoft and Sällfors (2003).

In the reference case we use the following functions and data:

$$\begin{aligned} &k(S) = k(1) \cdot S^3, \qquad k(1) = 1.6 \cdot 10^{-20}, \qquad \lambda(S) = 0.6 + 0.6 \cdot S \ \ \mathrm{W/(mK)}, \\ &D_\mathrm{v}(S) = (1-S) \cdot D_\mathrm{v}(0), \qquad D_\mathrm{v}(0) = 2 \cdot 10^{-6} \ \ \mathrm{m^2/s} \qquad S_\mathrm{in} = 0.85, \qquad V_\mathrm{p} = 0.39. \end{aligned} \tag{3.6}$$

The chosen type of functions and data for bentonite are those of Rutquist, Noorishad and Tsang (1999).

3.3 General form for flow equations

The moisture flux g and the conductive-convective heat flux q may now be written in the following general form

$$g(r,t) = -K_S(S,T) \cdot \frac{\partial S}{\partial r} - K_T(S,T) \cdot \frac{\partial T}{\partial r}. \tag{3.7}$$

$$q(r,t) = -\lambda_S(S,T) \cdot \frac{\partial S}{\partial r} - \lambda_T(S,T) \cdot \frac{\partial T}{\partial r}. \tag{3.8}$$

The flow coefficients for moisture, K_S and K_T, and for heat, λ_S and λ_T, are functions of the state variables S and T. For K_S and K_T we have:

$$K_S(S,T)=\left(\frac{\rho_{\mathrm{w}}k(S)}{\eta(T)}+D_{\mathrm{v}}(S)\cdot\frac{\partial\rho_{\mathrm{v}}}{\partial P}\right)\cdot\frac{dP}{dS}. \tag{3.9}$$

$$K_T(S,T)=K_T'(S)\cdot(1-S), \qquad K_T'(S)=D_{\mathrm{v}}(0)\cdot\frac{\partial\rho_{\mathrm{v}}}{\partial T}. \tag{3.10}$$

The function $K_T(S,T)$ involves the factor $1-S$ from the vapor diffusivity (3.4). This factor is zero for $S=1$, when the gas phase has vanished. The remaining flow coefficient $K_T'(S,T)$ is has a very much smaller variation with *S* and *T*. The coefficient functions are readily calculated in the mathematical program.

3.4 Temperature over the bentonite annulus

The total heat release from the canister is $Q_{\mathrm{c}}(t)$ (W). It varies in time with a time scale of years. The time scale to establish a steady-state temperature profile over the bentonite annulus is below 24 hours. We may therefore with very good accuracy consider the temperature as quasi steady state or independent of time. But the value of Q_{c} and the temperature level and profile in the bentonite will vary slowly with time. In any particular moderate time span, we have a constant value of Q_{c} and a constant temperature T_{r} at the rock boundary. The radial temperature profile $T(r)$ satisfies, using (3.3) and (3.2) without the convective terms, the heat balance equation

$$Q_c=-2\pi rH_{\mathrm{c}}\cdot\lambda(S)\cdot\frac{\partial T}{\partial r}, \qquad T(r_{\mathrm{r}})=T_{\mathrm{r}}. \tag{3.11}$$

The solution $T(r)$ depends on Q_{c}, T_{r} and the thermal conductivity $\lambda(S)$ over the annular region.

3.5 Thermo-diffusive coefficient function A(S,T)

The moisture flux *G*, (3.3) and (3.7), may be written in an alternative form that will prove to be very useful for our analysis. We eliminate the temperature gradient by using (3.11). We also use (3.10). Then we may write the flux in the following way

$$G=-2\pi H_{\mathrm{c}}\cdot K_S(S,T)\cdot\left[r\cdot\frac{\partial S}{\partial r}-2\cdot A(S,T)\cdot(1-S)\right] \tag{3.12}$$

The first part is of a diffusive character, and the second one of a convective character with a flow coefficient function times $1-S$. Here, we have introduced the thermo-diffusive coefficient function $2\cdot A(S,T)$ as the ratio between the functions before $1-S$ and $r\cdot\partial S/\partial r$. We have

$$A(S,T)=\frac{K_T'(S,T)}{4\pi H_{\mathrm{c}}\cdot K_S(S,T)}\cdot\frac{Q_{\mathrm{c}}}{\lambda(\mathrm{S})}. \tag{3.13}$$

The factor 2 is introduced in order to have convenient notations.

The thermo-diffusive coefficient function $A(S,T)$ is of a somewhat intricate character. The first right-hand factor is the ratio between the reduced coefficient K_T', where the factor $1-S$ is taken away, and K_S. The second factor involving the heat emission represents the temperature gradient in accordance with (3.11).

3.6 Moisture balance equation

The moisture balance equation for the degree of water saturation $S(r,t)$ in the pores of the bentonite in the considered radial, time-dependent case for an annular bentonite region between canister and rock walls is

$$\frac{\partial}{\partial t}\left[2\pi r H_\mathrm{c} \cdot V_\mathrm{p}\rho_\mathrm{w} S\right] = -\frac{\partial G}{\partial r}, \qquad r_\mathrm{c} < r < r_\mathrm{r},$$

or, using (3.12),

$$V_\mathrm{p}\rho_\mathrm{w} \cdot \frac{\partial S}{\partial t} = \frac{1}{r}\cdot\frac{\partial}{\partial r}\left\{K_S(S,T)\cdot\left[r\cdot\frac{\partial S}{\partial r} - 2A(S,T)\cdot(1-S)\right]\right\}, \qquad r_\mathrm{c} < r < r_\mathrm{r}. \qquad (3.14)$$

Here, V_p is the porosity or pore volume per unit volume of bentonite, and H_c the height of the canister.

The above equation involves a diffusivity function $K_S/(V_\mathrm{p}\rho_\mathrm{w})$ and the thermo-diffusive function. We have arrived at the equation

$$\frac{\partial S}{\partial t} = \frac{1}{r}\cdot\frac{\partial}{\partial r}\left\{D(S,T)\cdot\left[r\cdot\frac{\partial S}{\partial r} - 2\cdot A(S,T)\cdot(1-S)\right]\right\}, \qquad r_\mathrm{c} < r < r_\mathrm{r}. \qquad (3.15)$$

The moisture diffusivity $D(S,T)$ (m^2/s) and the flow coefficient function $A(S,T)$ (-) are given by

$$D(S,T) = \frac{K_S(S,T)}{V_\mathrm{p}\rho_\mathrm{w}}, \qquad A(S,T) = \frac{Q_\mathrm{c}(t)}{4\pi H_\mathrm{c}}\cdot\frac{K_T'(S,T)}{K_S(S,T)\cdot\lambda(S)}. \qquad (3.16)$$

We obtain a *single* equation (3.15) for $S(r,t)$. Any variation of the temperature profile with time is determined from (3.11) with a very slowly varying $Q_\mathrm{c}(t)$ and $T_\mathrm{r}(t)$. The second term involving $1-S$ is caused by the water vapor diffusion due to the temperature gradient.

4. Steady-state analyses

As mentioned above, the time scale to approach (exponentially) steady-state moisture conditions is around 4 years in the wet-rock case, and around 1 year in the dry-rock case for the reference data. The temperature and the heat release from the canisters have a distinctly longer time scale. *Steady-state* solutions for the moisture distribution over the bentonite annulus are therefore quite interesting to us. The steady-state solutions are discussed in more detail in the report Claesson, Hagentoft and Sällfors (2003).

4.1 General steady-state equations

The general steady-state relations are given by (3.7) and (3.8). The fluxes G and Q, (3.3) are independent of the radius r in steady state. The moisture flux is zero, since it is zero at the canister boundary. We have

$$G = 0, \qquad Q = Q_{\mathrm{c}}(t). \tag{4.1}$$

From (3.7), (3.8), (3.3) and (4.1), we get an equation system for the derivatives dS/dr and dT/dr. From this equation system we get the derivatives. We have:

$$\frac{dS}{dr} = -\frac{Q_c(t)}{2\pi rH} \cdot \frac{K_T(S,T)}{K_T\lambda_S - K_S\lambda_T},$$

$$\frac{dT}{dr} = \frac{Q_c(t)}{2\pi rH} \cdot \frac{K_S(S,T)}{K_T\lambda_S - K_S\lambda_T}, \qquad r_{\mathrm{c}} \le r \le r_{\mathrm{r}}. \tag{4.2}$$

The four flow coefficients are functions of S and T. We have two coupled, strongly nonlinear, ordinary differential equations for $S(r)$ and $T(r)$. We study the solution for any value of S and T at the rock boundary $r = r_{\mathrm{r}}$:

$$S(r_{\mathrm{r}}) = S_{\mathrm{r}}, \qquad T(r_{\mathrm{r}}) = T_{\mathrm{r}}(t). \tag{4.3}$$

Let us first consider the *wet-rock case* with full saturation at the rock boundary: $S(r_{\mathrm{r}}) = 1$. The flow function $K_T(S,T)$ involves the factor $1-S$, (3.10). This means that the value of K_T and the derivative dS/dr, (4.2) top, is zero for $S = 1$. From this it follows for the steady-state wet-rock case:

$$K_T(1,T) = 0, \qquad S(r_{\mathrm{r}}) = 1 \;\Rightarrow\; S(r) = 1, \qquad r_{\mathrm{c}} \le r \le r_{\mathrm{r}}. \tag{4.4}$$

The full saturation at the rock boundary is always imposed throughout the bentonite after an initial drying at the canister side. The time scale for this saturation is around 4 years in the reference case.

The situation is very different in the *dry-rock case* (or in a case with partial saturation only at the rock boundary, $S(r_{\mathrm{r}}) = S_{\mathrm{r}} < 1$). We will see below that then we always get drying at the canister side. I the rest of this section we consider the dry-rock case.

4.2 Coordinate-independent relation between *S* and *T*

There is a specific, quite useful, internal structure in the differential equations (4.2) for $S(r)$ and $T(r)$. We divide the first equation by the second one. The differential *dr* and all factors except the *K*-functions cancel. We have in the temperature interval from the rock temperature T_{r} to the higher temperature T_{c} at the canister

$$\frac{dS}{dT} = -\frac{K_T(S,T)}{K_S(S,T)}, \qquad T_{\mathrm{r}} \le T \le T_{\mathrm{c}}. \tag{4.5}$$

The relation between *S* and *T* becomes *independent* of the radius *r*. The temperature T_{c} at the canister boundary is obtained integration of the steady-state formula (3.11) (using a suitable average saturation):

$$T_{\mathrm{c}} \approx T_{\mathrm{r}}(t) + \frac{Q_c(t)}{2\pi H \cdot \lambda(S_{\mathrm{av}})} \cdot \ln\left(\frac{r_{\mathrm{r}}}{r_{\mathrm{c}}}\right). \tag{4.6}$$

4.3 Solution for the reference case

In a reference case we take

$$Q_{\mathrm{c}} = 1000 \ \ \mathrm{W}, \qquad \mathrm{S_r} = 0.95, \qquad T_{\mathrm{r}} = 70 \ {}^{\mathrm{o}}\mathrm{C}. \tag{4.7}$$

We choose a rather high value for S_{r} in order to avoid large drying.

The equations (4.2) for $S(r)$ and $T(r)$ are solved with the program Mathcad. The computer calculations take a few seconds only. The results, $S(r)$ and $T(r)$, are shown in Fig. 4.1. The saturation falls from S=0.95 at the rock to 0.83 at the canister, while the temperature increases inwards from 70 to 81.8 ˚C. There is a clear but moderate drying of the bentonite in the reference case. The approximation (4.6) gives the canister temperature 70+11.3=81.3. It underestimates the temperature difference over the bentonite by 5%.

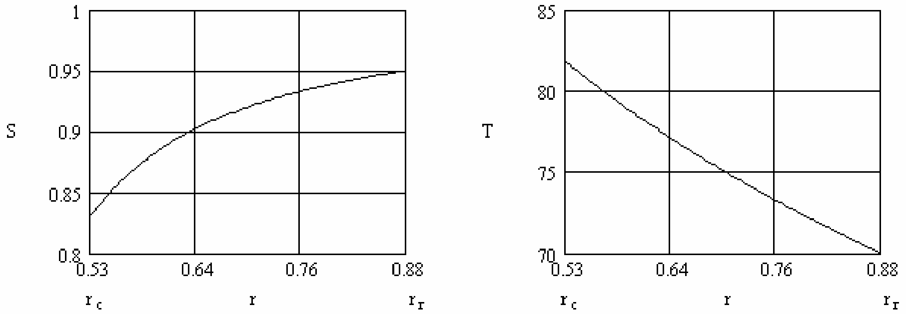

Figure 4.1. Degree of water saturation $S(r)$ and temperature $T(r)$ for the reference case.

4.4 Charts for S(T)

The differential equation for the coordinate-independent relation between S and T, (4.5), is discussed in Section 4.2. We will here give a complete chart for these relations for the reference case. We will also illustrate the importance of the magnitude of the conductivity ratio by varying $D_{\mathrm{v}}(0)$.

A suitable number of initial saturation degrees are chosen. We have the mathematical problem:

$$\begin{aligned} &\frac{dS}{dT} = -\frac{K_T(S,T)}{K_S(S,T)}, \qquad T_{\min} \le T \le T_{\max}, \\ &S(T_{\min}) = S_1,\ S_2, ..., \qquad 1 > S_1 > S_2 > ... > 0. \end{aligned} \tag{4.8}$$

We take the interval $20 \le T \le 100$ ˚C in order to cover all normal applications. The start values at $T = T_{\min}$ are S = 0.4, 0.5, … 0.995, and 0.999. The set of curves or chart is shown in Fig. 4.2.

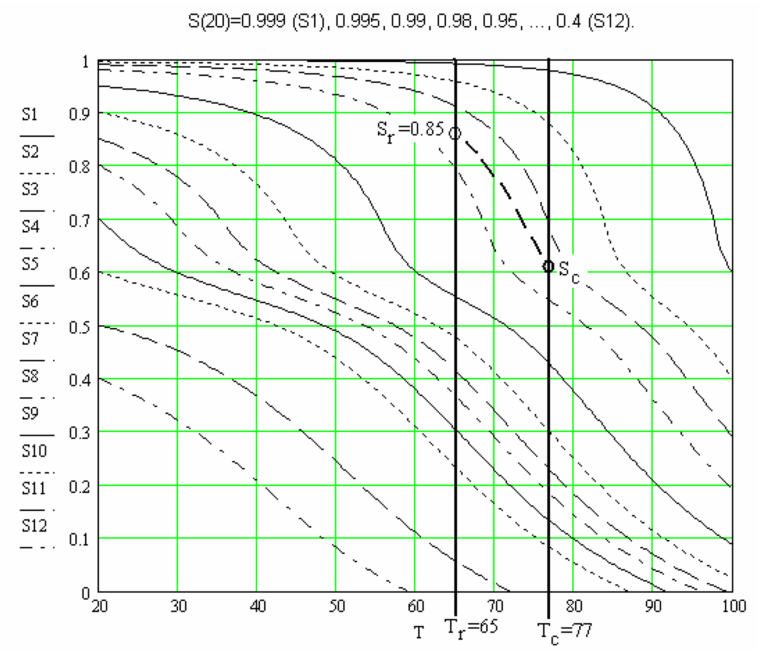

Figure 4.2. Set of curves $S(T)$ to cover all cases in $20 \le T \le 100$ ˚C for the reference case.

The charts are used in the following way. We have a prescribed rock temperature T_r and a prescribed degree of saturation S_r. This point is marked in the chart in Fig. 4.2. We choose the nearest curve on the vertical line $T = T_\mathrm{r}$ or the two curves above and below. The solution will follow this curve or lie between the two enclosing curves. We need to know the upper temperature T_c. A good estimate is given by (4.6). An example is shown in Fig. 4.2: $T_\mathrm{r} = 65$ and $S_\mathrm{r} = 0.85$. We estimate T_c to 77 ˚C from (4.6). We will follow the indicated curve between S3 and S4. The chart is *a very handy way* to estimate the drying.

4.5 Linearized equation for S(r)

The equation for the steady-state solution $S(r)$ becomes from (3.12)

$$r \cdot \frac{dS}{dr} - 2 \cdot A(S,T) \cdot (1-S) = 0, \qquad r_\mathrm{c} \le r \le r_\mathrm{r}. \tag{4.9}$$

A particular solution is $S(r) = 1$ for all r. This is the solution in the wet-rock case with $S(r_\mathrm{r}) = 1$. In the *dry-rock case,* which is considered from now on in this section, we get a moisture distribution from dry to wet over the annular region.

A linerization of the equation for the degree of saturation S is discussed in Section 5. We will here consider this linerization in the steady-state case. We make as in (5.1) the approximation

$$A(S,T) \approx A(S_0,T_0) = a. \tag{4.10}$$

Here, S_0 is a mean water saturation level and T_0 the mean temperature in the bentonite for the considered case. The total moisture content, which is given by the integral of $2\pi r H_\mathrm{c} \cdot S$ over $r_\mathrm{c} \le r \le r_\mathrm{r}$, must be the same for $S = S(r)$ and for $S = S_\mathrm{in}$ (initial value) in the dry-rock case. We have to solve (4.9) with the approximation (4.10) and an integral relation. The solution is:

$$S_{\mathrm{ss}}(r) = 1-(1-S_{\mathrm{in}})\cdot\frac{1-a}{1-s_{\mathrm{c}}^{2-2a}}\cdot\frac{1-s_{\mathrm{c}}^{2}}{(r/r_{\mathrm{r}})^{2a}}, \qquad r_{\mathrm{c}} \le r \le r_{\mathrm{r}}, \qquad \left(s_{\mathrm{c}} = r_{\mathrm{c}}/r_{\mathrm{r}}\right). \tag{4.11}$$

Figure 4.3 shows the steady-state moisture distribution (4.11) for the reference value $S_{\mathrm{in}} = 0.85$ for different values of a. This curves give the *largest* drying that may occur in the bentonite.

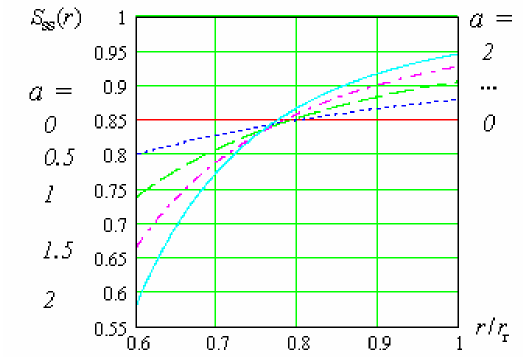

Figure 4.3. Steady-state moisture distribution (4.11) for $S_{\mathrm{in}} = 0.85$ for different values of a in the dry-rock case. It gives the largest drying that may occur in the bentonite.

We are in particular interested in the largest drying at the canister wall, $S_{\mathrm{ss}}(r_{\mathrm{c}})$. We have

$$S_{\mathrm{ss}}(r_{\mathrm{c}}) = 1-(1-S_{\mathrm{in}})\cdot\frac{1-a}{s_{\mathrm{c}}^{2a}-s_{\mathrm{c}}^{2}}\cdot\left(1-s_{\mathrm{c}}^{2}\right), \qquad a \ne 1. \tag{4.12}$$

Figure 4.4 shows this largest drying, which may occur in the bentonite as a function of a for different initial degrees of water saturation S_{in} in the bentonite. The curves start at $S_{\mathrm{ss}}(r_{\mathrm{c}}) = S_{\mathrm{in}}$ for $a = 0$, and they decrease with a larger drying as a increases.

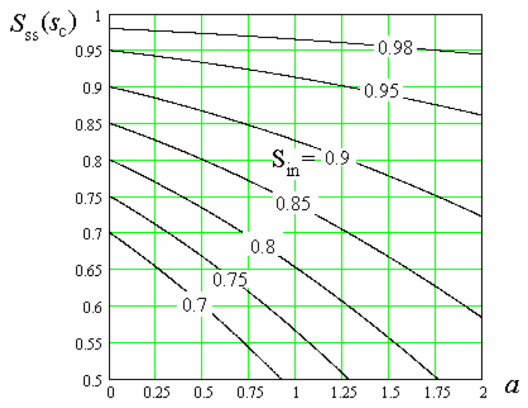

Figure 4.4. Steady-state moisture distribution (4.12) at the canister wall as a function of a for different initial degrees of water saturation S_{in} in the bentonite. These curves give the largest drying that may occur in the bentonite.

5. Assessing drying, wetting and resaturation

The highly non-linear equation (3.15) for the saturation $S(r,t)$ may be linearized with certain loss of accuracy. In this approximation, new analytical solutions for the time-dependent radial water flow process through the bentonite annular region have been derived for the dry-rock and wet-rock cases. They involve Bessel functions and Fourier expansion technique. The results for the wet-rock case are presented in detail in Claesson, 2003A and 2003B. From this it is possible to give explicit formulas for the intensity and time scale of the drying, and for the time scale of the water resaturation process in the wet-rock case.

5.1 Linearization of the equation for S(r,t)

The general moisture balance equation for $S(r,t)$, (3.14), involves the moisture diffusivity function $D(S,T)$ and thermo-diffusive parameter $A(S,T)$ These functions depend on the flow properties of the bentonite with its water in the pores, (3.16) and (3.9)-(3.10). The two functions are shown in Figs. 5.1-2 for the reference data. They are calculated with a Mathcad program.

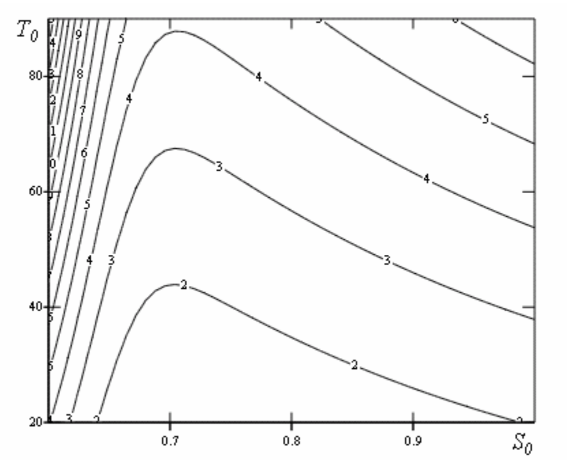

Figure 5.1. Diffusivity function $D(S_0,T_0)\cdot 10^{10}$ (m^2/s) using reference bentonite data.
Intervals for saturation and temperature: $0.6 \le S_0 \le 1,\ 20 \le T_0 \le 90^{\circ}\,\mathrm{C}$.

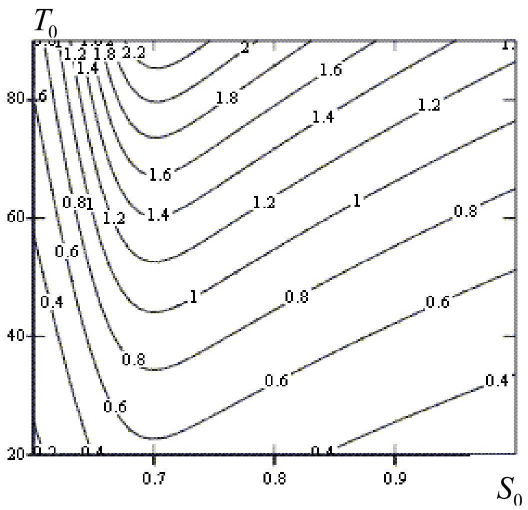

Figure 5.2. The thermo-diffusive function $A(S_0,T_0)$ using reference bentonite data.
Intervals for saturation and temperature: $0.6 \le S_0 \le 1,\ 20 \le T_0 \le 90\ ^{\circ}\mathrm{C}$.

Consider as an example the variation of $D(S,T)$ and $A(S,T)$ in the region 0.8<S<1 and 70<T<80°C. There is a variation of some $\pm 20\%$. This is quite typical for the type of cases that we will consider. It may be noted that the factor $1-S$ varies much more (by a factor 20 between S=0.8 and S=0.99). This separation of the factor $1-S$ is the key idea to obtain a tractable problem.

The drying and wetting process will in the cases we consider have a variation of the flow coefficients $D(S,T)$ and $A(S,T)$ in the governing equation (3.14) of up to $\pm 20\%$. We may with some caution approximate the two functions by suitable *constant mean values*:

$$D(S,T) \approx D(S_0,T_0) = D_0, \qquad A(S,T) \approx A(S_0,T_0) = a. \tag{5.1}$$

Here, S_0 is a mean saturation level and T_0 the mean bentonite temperature the for the considered case.

We introduce these approximations in (3.15). The error involved in this approximation is judged to be below 10 %, since the flow functions have values both above and below the approximate constant values. There are now two parameters in(3.15). We get a mean effective diffusivity D_0 and a convective-diffusive parameter a from the dimensionless factor before $1-S$:

$$D_0 = \frac{K_S(S_0,T_0)}{V_{\mathrm{p}}\rho_{\mathrm{w}}}, \qquad a = \frac{Q_{\mathrm{c}}}{4\pi H_{\mathrm{c}}} \cdot \frac{K_T'(S_0,T_0)}{K_S(S_0,T_0)\lambda(S_0)}. \tag{5.2}$$

Equation (3.15) with the approximations (5.1) may now be written

$$\frac{1}{D_0} \cdot \frac{\partial S}{\partial t} = \frac{1}{r} \cdot \frac{\partial}{\partial r}\left[r \cdot \frac{\partial S}{\partial r} - 2a \cdot (1-S) \right], \qquad r_{\mathrm{c}} < r < r_{\mathrm{r}}. \tag{5.3}$$

The initial degree of saturation in the bentonite is S_{in}. The moisture flux is zero at the canister boundary. At the rock boundary $r = r_{\mathrm{r}}$, the moisture flux zero in the dry-rock case, , while full saturation S=1 is maintained in the wet-rock case. Equation (5.3) for $S(r,t)$ in a slightly modified form together with initial and boundary conditions give the following problem for $S(r,t)$:

$$\frac{1}{D_0} \cdot \frac{\partial S}{\partial t} = \frac{\partial^2 S}{\partial r^2} + \frac{1+2a}{r} \cdot \frac{\partial S}{\partial r}, \qquad r_{\mathrm{c}} < r < r_{\mathrm{r}}; \tag{5.4}$$

$$S(r,0) = S_{\mathrm{in}}, \qquad r_{\mathrm{c}} < r < r_{\mathrm{r}}; \tag{5.5}$$

$$r = r_{\mathrm{c}}: \quad r_{\mathrm{c}} \cdot \left.\frac{\partial S}{\partial r}\right|_{r=r_{\mathrm{c}}} = 2a\left[1 - S(r_{\mathrm{c}},t)\right]; \tag{5.6}$$

$$\begin{aligned} r = r_{\mathrm{r}}: \quad &\text{Dry-rock case:} \quad r_{\mathrm{r}} \cdot \left.\frac{\partial S}{\partial r}\right|_{r=r_{\mathrm{r}}} = 2a \cdot \left[1 - S(r_{\mathrm{r}},t)\right], \\ &\text{Wet-rock case:} \quad S(r_{\mathrm{r}},t) = 1. \end{aligned} \tag{5.7}$$

The problem (5.4)-(5.7) for $S(r,t)$ involves one essential parameter *a* only. Time is scaled with the diffusivity factor D_0. The solution $S(r,t)$ is expressed with dimensionless radius s and time τ:

$$s = r/r_{\mathrm{r}}, \qquad \tau = t/t_0, \qquad t_0 = \frac{4(r_{\mathrm{r}} - r_{\mathrm{c}})^2}{\pi^2 D_0}. \tag{5.8}$$

Here, we have introduced a suitable *basic time scale* t_0.

5.2 An example. The reference case

The two above solutions have been implemented in the mathematical computer program Mathcad. The solutions are readily calculated in any particular case requiring moderate computer time. In this example and in all other examples, we have $s_{\mathrm{c}} = r_{\mathrm{c}}/r_{\mathrm{r}} = 0.6$.

For the examples in this section, we take

$$a = 0.9, \qquad S_{\mathrm{in}} = 0.85. \tag{5.9}$$

The value *a*=0.9 corresponds to $S_0 = 0.9$ and $T_0 = 60$ °C in Fig. 7.2.

5.2.1. Dry-rock case

The degree of water saturation *S* is shown in Fig. 5.3 as a function of r/r_{r} for different dimensionless times $\tau = t/t_0$. The initial value at zero time is $S = 0.85$. We see a drying at the warm canister side and a wetting on the colder rock side, both of which increase with time. The total water content is constant in time, since moisture flux is zero at both boundaries. The solution approaches the steady-state moisture distribution $S_{\mathrm{ss}}(s)$, (4.11). It is quite close for $t/t_0 = 0.8$.

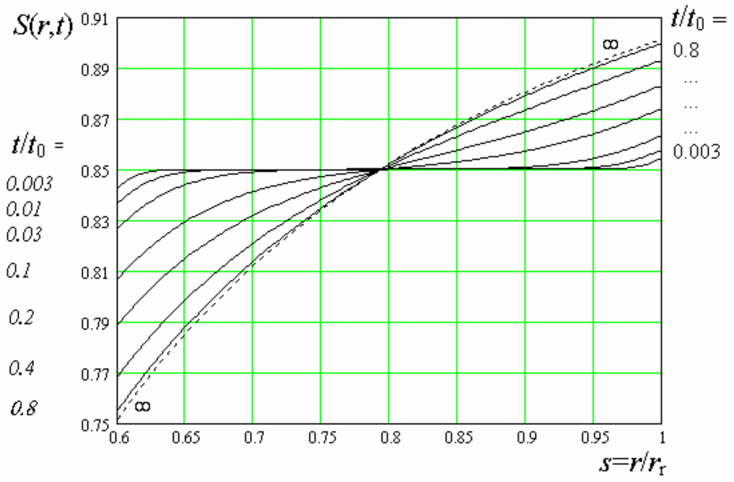

Figure 5.3. The degree of saturation $S(r,\tau)$, $r_{\mathrm{c}}/r_{\mathrm{r}} \le r/r_{\mathrm{r}} \le 1$, for a=0.9.

The strongest drying occurs at the warm canister boundary $r = r_{\mathrm{c}}$. Fig. 5.4 shows the drying from the initial value S_{in} to the final largest drying $S_{\mathrm{ss}}(r_{\mathrm{c}}) = 0.752$ at steady state (a=0.9 in Fig. 4.3).

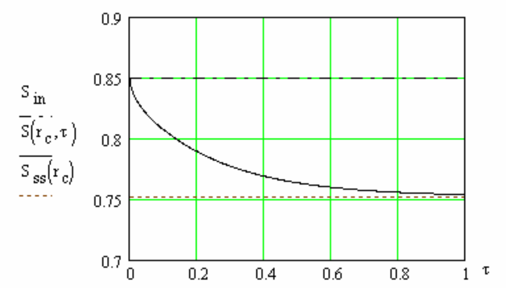

Figure 5.4. Degree of saturation $S(r_c,\tau)$ at the canister boundary, where the strongest drying occurs.

5.2.2 Wet-rock case

The calculated drying, wetting and resaturation process is shown in Fig. 5.5 in the wet-rock case. The curve for the shortest time τ=0.002 shows a small drying near the canister, and increased saturation from the initial value *S*=0.85 to *S*=1 in a small region near the rock boundary, where full saturation $S=1$ is maintained. The intermediate region is unchanged. The dried region and the region of increased saturation both increase in time. Water from the dried region is displaced by vapor diffusion through the undisturbed intermediate region to the outer parts. At $\tau \approx 0.05$, the two regions meet at $r/r_r \approx 0.8$. The drying in the inner region continues until the time of largest drying τ= 0.216. Then the wetting process becomes dominant also at the canister wall. There is from this time a steady wetting of all the bentonite. The initial saturation at the canister wall (*S*=0.85) is restored at the time τ= 0.694.

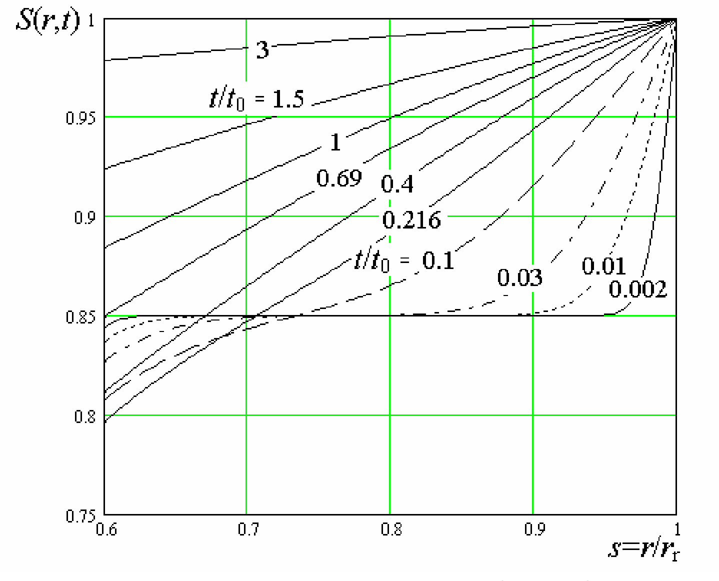

Figure 5.5. The degree of saturation $S(r,\tau)$, $r_c/r_r \le r/r_r \le 1$, for a=0.9. Maximum drying at τ = 0.216. Initial saturation S=0.85 is recovered at canister wall for τ= 0.69.

The strongest drying occurs at the warm canister boundary $r=r_c$. Fig.5.6 shows the degree of saturation at the canister boundary as function of time. There is an initial drying with the minimum saturation $S = 0.79$ for $\tau = 0.216$. From that time there is a steady increase up to full saturation at, say, $\tau = 5$.

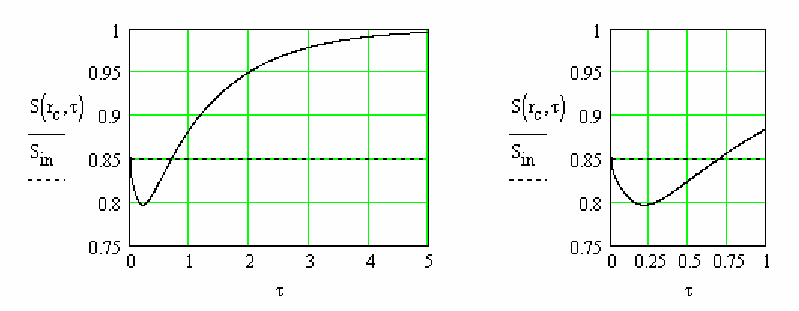

Figure 5.6. Degree of saturation $S(r_c, \tau)$ at the canister boundary, where the strongest drying occurs.

5.3 Dependence on saturation and temperature level

The above solution involves the two key parameters t_0 and *a*. The time scale t_0 is essentially the inverse of D_0, (5.8). The basic parameters D_0 and *a* are defined in (5.2). They depend on the choice of average saturation level S_0 and average temperature level T_0. The functions $D_0 = D(S_0, T_0)$ and $a = A(S_0, T_0)$ are shown in Figs. 5.1 and 5.2 for the reference data.

For the time scale t_0, we have from (5.8) and (5.2):

$$t_0 = \frac{4(r_\mathrm{r} - r_\mathrm{c})^2}{\pi^2 D_0}, \qquad t_{0\mathrm{y}}(S_0, T_0) = \frac{4(r_\mathrm{r} - r_\mathrm{c})^2 \cdot V_\mathrm{p} \rho_\mathrm{w}}{\pi^2 \cdot K_S(S_0, T_0) \cdot t_\mathrm{y}}. \tag{5.10}$$

The function $t_0(S_0, T_0)$ is divided by the time of a year t_y = 3600·24·365 s, which means that $t_{0\mathrm{y}}$ is the time scale in years. Figure 5.7 shows $t_{0\mathrm{y}}(S_0, T_0)$ for the reference data. The Mathcad program generates such a plot in no time for any bentonite (and water) data.

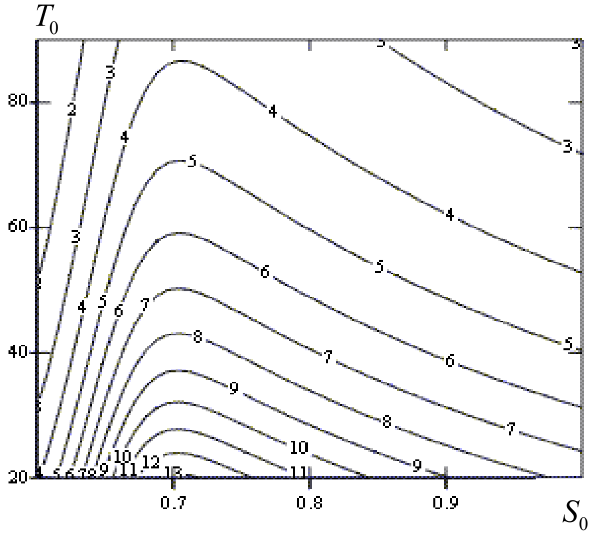

Figure 5.7. The time scale $t_{0\mathrm{y}}(S_0,T_0)$ using reference bentonite data. Intervals in degree of saturation and temperature: $0.6 \le S_0 \le 1$, $20 \le T_0 \le 90\ ^{\mathrm{o}}\mathrm{C}$.

The time scale t_0, (5.10), is determined by the average diffusivity D_0, or by $K_S(S_0,T_0)$. The dimensionless parameter *a*, (5.2), is proportional to the heat flux Q_c / H. It is also proportional to the ratio between the reduced flow coefficient $K_T'(S_0,T_0)$ for the temperature and the flow coefficient $K_S(S_0,T_0)$ for saturation gradients. It is a thermo-diffusive parameter. It should be noted that the time scale t_0 is inversely proportional to the flow coefficient K_S, while *a* only depends on the ratio between the two basic flow coefficients.

6. Key parameters and sensitivity analysis

A sensitivity analysis is presented in Claesson, Hagentoft and Sällfors (2003). These results are not reported here again.

We have seen that the potential drying depends on the two parameters a and t_0 only. The two parameters depend in turn on the flow properties of bentonite, on the temperature level and gradient, and on properties of water. We will here present a rule of thumb to assess the key factors.

6.1 Key factors for the thermo-diffusive parameter a

The parameter a is defined by (5.2). It is proportional to the various key factors in the following way:

$$a \propto \frac{Q_\mathrm{c}}{H_\mathrm{c}}, \quad a \propto \frac{1}{\lambda(S_0)} \approx \frac{1}{\lambda(1)}, \quad a \propto K_T'(S_0,T_0) \propto D_\mathrm{v}(0), \quad a \propto \frac{1}{K_S(S_0,T_0)} \propto \frac{1}{k(1)}. \qquad (6.1)$$

In the third proportionality, (3.10) is used. In the fourth one, (3.9) is used. Here, the last proportionality giving $1/k(1)$ may in case of doubt be tested with model that gives $A(S,T)$. The factors above show how a depends on four key factors. Let us define the key product *f* as

$$f = \frac{Q_\mathrm{c}}{H_\mathrm{c}\lambda(1)} \cdot \frac{D_\mathrm{v}(0)}{k(1)}, \qquad f_\mathrm{ref} = \left(\frac{Q_\mathrm{c}}{H_\mathrm{c}\lambda(1)} \cdot \frac{D_\mathrm{v}(0)}{k(1)} \right)_\mathrm{ref}. \qquad (6.2)$$

Here, a_ref is the *a*-value in the reference case.

A rule of sum to *assess the variation* of a with the key factors is now

$$a \approx \frac{f}{f_\mathrm{ref}} \cdot a_\mathrm{ref}. \qquad (6.3)$$

This means that a is doubled, when the vapor diffusivity for bentonite $D_\mathrm{v}(0)$ or the heat flux Q_c is doubled. The parameter a is approximately doubled, when thermal conductivity of fully saturated bentonite $\lambda(1)$ or the hydraulic conductivity of fully saturated bentonite $k(1)$ is halved.

6.2 Key factors for the time scale t_0

The basic time scale t_0 is inversely proportional to the mean diffusivity D_0, (5.8), which is proportional to $K_S(S_0,T_0)$, (5.2). We have as in (6.1), right,

$$t_0 \propto \frac{1}{D_0} \propto \frac{1}{K_S(S_0,T_0)} \propto \frac{1}{k(1)}. \tag{6.4}$$

As a rule of thumb we have that the key factor to determine the basic time scale is the inverse of $k(1)$:

$$t_0 \approx \frac{k(1)|_{\text{ref}}}{k(1)} \cdot t_{0,\text{ref}}. \tag{6.5}$$

Here, $t_{0,\text{ref}}$ is the value in the reference case. The time scale decreases by a factor 10, when $k(1)$ is increased by a factor 10.

7. Survey of models

A number of small computer models has been developed as handy tools of analysis to understand and assess the potential drying under various conditions. All models are implemented in Mathcad. The models, which consist of a moderate set of formulas and computations, should be reasonable straight forward to implement in other mathematical programs such as Matlab or Maple.

1. General steady-state solution for S(r) and T(r).
2. Chart for S(T).
3. Key parameters D, A and t_{0y} as functions of S and T.
4. Solution S(r,t) in dry-rock case.
5. Solution S(r,t) in wet-rock case.

Explicit, quite accurate Formulas for water and bentonite are used in the first three models.

8. Conclusions

The aim of this study has been to develop tools of analysis to assess the drying of the bentonite. A few small models based on a number of equations are available in Mathcad. They should be quite easy to translate to other mathematical programs.

The key parameters are a time scale t_0 and a thermo-diffusive parameter a. These depend in a rather complicated way on flow properties of bentonite, properties of water, level of degree of water saturation and temperature in the bentonite annulus, and on the temperature gradient. But they are readily calculated with the models.

At the outer boundary $r = r_{\text{r}}$, there are two limits. The rock may be sufficiently wet to maintain full saturation at the surface of the bentonite, the wet-rock case. The other limit, which is the worst possible case, is that the water flow from the rock is zero, the dry-rock case.

The bentonite will always start to dry at the warmer canister side (except for case of full saturation initially when nothing happens), and the saturation will increase on the rock side from the initial saturation S_{in}. In the wet-rock case, wetting from the fully saturated rock side will stop the drying after a certain time, and a successive wetting of all bentonite continues toward full saturation in the whole annulus after, say, $3 \cdot t_0$, Fig. 5.5. In the dry-rock case, drying on the canister side and wetting on the rock side continue until a steady-state moisture distribution is established, Fig. 5.3. Then water vapor flow outwards and liquid water flow inwards balance each other at all points in the bentonite.

The curves in Figs. 5.3 and 5.5 show drying in the left-hand half of $r_c \le r \le r_r$, and wetting above $S = S_{in}$ in the right-hand half of the interval. This is a general feature. This means that the outer half of the bentonite annulus *never dries below* the initial degree of water saturation S_{in}. The strongest drying occurs in a rather thin layer near the canister.

The steady-state moisture distributions, which are attained after the time t_0 in the dry-rock case, are analyzed in detail. Models for the exact moisture profiles are available. A handy tool is a chart for the coordinate-independent relations $S = S(T)$.

The steady-state solutions are simplified in the linearized case. We get very handy formulas to assess the largest drying. Formula (4.12) and Fig. 4.4 give the largest possible drying as function of the two parameters S_{in} and a, only.

The complete process is obtained for any a-value in the linearized case from new analytical solutions. Then we also have formulas and graphs that give the drying at the canister side.

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STUK'S VIEW ON BUFFER AND BACKFILL ISSUES

REVIEW OF POSIVA'S RTD PROGRAMME TKS-2003.

Jussi Heinonen, STUK

General

This presentation gives an idea of STUK's responsibilities and situation towards Government and Posiva. Also the time table of the Finnish programme is given. STUK's view and most of the comments related to buffer and backfill issues are from STUK's review of Posiva's RTD programme, which was carried out this year (2004) with the help of the External Review Group.

In short the key organisations for regulatory functions presented as follows:

- The Government grants licenses for nuclear facilities and issues general safety regulations.
- The Ministry of Trade and Industry (MTI) oversees that implementation of waste management and related R&D complies with the national policy and, together with the State Nuclear Waste Management Fund, that provisions for future waste management are adequate.
- STUK is responsible for the control of radiation and nuclear safety, for issuing detailed safety regulations and for the technical and safety related review of licence applications and other important documents.

The spent fuel disposal programme is subject to regulatory oversight by the MTI and STUK. The main regulatory tools in the current preparatory phase have been mandatory regulations and triennial reviews of implementor's research, development and technical design programme (RTD). Construction and operation of the ONKALO (Underground Rock Characterisation Facility, URCF), which is envisaged to constitute a part of the disposal facility, is particularly subject to STUK's inspection and review activities.

Time schedule of the Finnish disposal programme

The Finnish spent fuel disposal has so far progressed in accordance with the target schedule established in the policy decision of 1983. A site screening report was published in 1985 and the site investigations started a couple of years later. Six sites have been subject to deep drillings and other surface based investigations, two of them being the NPP sites Olkiluoto and Loviisa. The final choice, involving e.g. environmental impact assessment (EIA) processes, was done between four sites. Of them, Posiva picked in 1999 the Olkiluoto site as the preferred disposal site.

The first authorisation step pursuant to the Finnish nuclear legislation is Government's Decision in Principle (DiP). In the DiP, the political and local acceptance for the nuclear project is requested and it is also crucial to siting the proposed nuclear facility. Posiva submitted its DiP application for building a spent fuel disposal facility at Olkiluoto in 1999. After STUK's positive safety appraisal, the proposed host municipality approved the application and the Finnish Government made the DiP in late 2000. Finally, the Parliament almost unanimously endorsed the DiP half a year later.

The next licensing step, pursuant to the nuclear legislation, is the construction license. According to the decision by the Ministry of Trade and Industry, the licence application should be submitted in 2012 at the latest. Currently Posiva is conducting an extensive research, development and technical design programme aiming at gaining preparedness for the submittal of the construction licence application. The programme includes site confirmation studies, technical design of the facilities and the engineered barrier system as well as development of safety assessment tools and databases.

After the Government has granted the construction licence, the encapsulation facility and the first compartments of the repository would be constructed. The operating licence process is scheduled to take place around 2020. The implementation of the spent fuel disposal facility and related regulatory control is detailed in Table 1.

Period	Implementation	Regulation
1983-1999	Technical design Site characterisation Research and development	Government's policy DiP of 1983 STUK's safety reviews of 1987, 1994 and 1997
1997-2001	EIA program and report DiP application for a disposal facility at Olkiluoto	EIA hearings and judgement STUK's preliminary safety appraisal Government's DiP and Parliaments endorsement
2000-2012	Site confirmation, incl. URCF Research, development and design	Oversight of site confirmation Triennial reviews of the program
2012-2019	Construction licence application Construction of the facilities	Review of licence application Oversight of construction
2020-	Operating licence application Operation of the facilities	Review of licence application Oversight of operation

STUK's RTD 2003 review

Posiva published in early 2004 on the request of the MTI the first RTD report (Posiva 2003) in a new series in research, development and technical design activities related to the management of radioactive waste. The report presents Posiva's RTD programme for spent nuclear fuel as well as the utilities RTD programmes for other nuclear waste being carried out by for the period of the subsequent three years.

STUK formed an External RTD Review Group in order to review the RTD report together with supporting technical and scientific reports Posiva's disposal studies. Three subgroups were formed so that the main areas of Posiva's RTD work could be covered. The three subgroups and their members are:

- Engineered barriers and facilities: Mick Apted (USA), Hannu Hänninen (Finland)
- Site characterisation and modelling: Ove Stephansson (Sweden /Germany), Juhani Suksi (Finland), Sven Tirén (Sweden)

- Research and assessment: David Read (UK), Peter Robinsson (UK), Chin-Fu Tsang (USA)

General comments

Posiva's programme has now entered a new phase, with the start of construction of ONKALO. This will be an interesting and intensive phase of work. The construction also sets a tight schedule for Posiva, which also implies a few issues. The completion of ONKALO is dated in 2010, which is two years before the licence submission. ONKALO should be a rock characterisation facility and in situ test place for Olkiluoto specific research or demonstration. However, few details are presented on in situ tests to be carried out in ONKALO. As noticed the time period between ONKALO completion and licence submission is short and it seems that the majority of tests that could help licensing will be performed during the construction period.

The structure of the RTD report and publication timetable were also under discussion. A recommendation was made for a more readable structure and for earlier publication by mid 2006. So that STUK would have time for review and feedback before the RTD period begins.

Main EBS findings

There were a few main findings in field of EBS. One obvious lack in Posiva's report/ programme is acceptance criteria. It is recommended that Posiva should define tentatively the acceptance criteria of the waste canister and buffer, taking account of the requirements arising from handling capability and long-term safety. The criteria should comply with the physico-chemical conditions around the canister and buffer. Also related inspection plans should be identified soon.

Another issue is that there is quite large number of open issues among different repository design components. In encapsulation and canister manufacturing, undecided issues include e.g. the site for encapsulation facility, the thickness of copper shell as well as the technique for manufacturing, closure and inspection of copper canister. The type of buffer material and its emplacement method are still under consideration. Undecided alternatives in disposal concept include vertical vs. horizontal deposition holes, one- or two-storey concept, and also the backfilling and closure methods for tunnels and shafts are still under consideration. At some point a decision will have to be made and the rationale for choosing one approach over alternatives explained. For STUK to be able to follow and understand these decisions bases (technical, operational, safety, cost) on which the decisions will be made and comparison tables for different alternatives are recommended to be formed.

In the report Posiva outlines the significance of the EBS for the long-term containment. Particularly canister is mentioned. Of course the host rock provides favourable and adequately predictable conditions which ensure the durability of waste canisters, and also provides the required complementary isolation in case the integrity of waste canisters is lost. The importance to safety of the barriers in various time periods should, however, be further specified e.g. in terms of quantitative performance targets and on that basis, an evaluation should be made, whether the weight of each sector in the RTD programme is in line with its relevance to safety.

KBS-3V vs. -3H

Posiva is developing, in co-operation with SKB, alternative disposal concept KBS-3H. The joint project has started in 2002 and is planned to end 2007. According to schedule drafting of safety assessment report for KBS-3H should start in 2007 and be published 2008. Similar report is planned for KBS-3V in 2007.

There are a few reasons why Posiva and SKB are developing this alternative:

- One or main reason might be difficulties with bentonite-aggregate backfill mixtures under high salinity conditions. With horizontal design these difficulties could be avoided or decreased.
- With horizontal design the inspectability of buffer-canister emplacement period would increase as the composition would be done in emplacement workshop.
- The reversibility of "super container" might be better than in the vertical concept (in case of canisters emplaced in non-compliant state).
- The sinking of the canister would be more improbable.
- The overall cost might be much lower for KBS-3H design.

A few additional concerns, that KBS-3H design raises are:

- A need for explorability of the host rock (higher likelihood of intersecting wet fractures).
- A re-consideration of the respect-distance concept to avoid major water-bearing fractures.
- Allowable straightness, surface roughness and wetted area to allow easy horizontal emplacement in tunnels.
- Development of new emplacement techniques.
- Evaluation if the combined EBS and near-field rock would behave similarly for KBS-3H as KBS-3V.

Buffer and backfill findings

Bentonite buffer has an important role especially in ensuring the performance of other engineered barriers. Bentonite has to attain favourable physical properties in re-saturation period and maintain them for long periods of time. Uncertainties in the performance of bentonite buffer involve long-term load bearing capability, yielding capability in rock movements, gas permeability and confirmation of uniform and timely re-saturation.

In RTD report Posiva mentions different aspects of buffer and backfill issues that have to be studied. However different tasks are given in bullet list and no explanation is done. More concrete plans or time tables would be needed. Posiva does not specify compaction method, pre-compacted buffer size, shape or even the type of bentonite. This gives an impression that future of buffer development is quite unclear.

Posiva's reference bentonite is a MX-80 bentonite for which considerable studies have been conducted. Posiva is now studying other bentonite types and possibly considering substituting MX-80 with another bentonite. The reason for this is not clear in RTD 2003. Certainly adopting a different bentonite will require significantly more detailed studies by Posiva, although other factors may favour this switch.

One concern raised in review is the post-emplacement inspectability of pre-compacted bentonite rings (i.e., are any unexpected gaps existing between rings). Open gaps, if persistent in the buffer, could allow direct and continuous contact of the copper by flowing groundwater containing oxidants. This would circumvent the slow diffusion-limited transport constraint of such oxidants through the buffer to the copper surface, which is the technical basis for the extremely long-lifetime (> 10^5 years) of copper canisters as established in the KBS-3 concept.

Posiva and SKB are developing alternative backfilling concepts to overcome the problem they have with high salinity ground water. A few reports concerning this development have been published. This quite basic development level (requirement specification, design development, feasibility study) in 2004-2005 raises a concern of adequate time. Especially in case of SKB there is no time to demonstrate that alternative backfill would work as designed.

EDZ

The excavation method used in construction of ONKALO, at least for the first part (~-260 m), is drill&blast method. Posiva has performed several studies for this and also for mechanical excavation methods in 2001-2003. The construction methods proposed are able to cause immediate centimetre to meter scale damage to the rock wall of the tunnels and deposition holes. The repository (thermal, swelling pressure) and environment (glaciation) can have effects on stresses in EDZ so that new or additional damage can be caused. The excavation-damaged zone around underground tunnels could have a significant impact, since it may become a continuous zone of relatively high permeability and porosity.

The reviewer’s opinion was that a programme of testing to characterise and evaluate the EDZ should be established. Methods to seal and interrupt the EDZ are proposed and these methods should be tested and demonstrated.

One uncertain issues related, at least partly, to EDZ is the present knowledge of the stress state. In Olkiluoto this uncertainty is a major weak point in the rock mechanics of the site. Posiva has carried out a few overcoring stress measurements, but some of them have suffered from microcracking after overcoring and therefore might not show the correct stress state.

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State-of-the-Art of Coupled Thermal-Hydrological-Mechanical Processes in the DECOVALEX Project

Lessons Learned and Important Issues

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INTRODUCTION

DECOVALEX (DEvelopment of COupled models and their VALidation against EXperiments in nuclear waste isolation) is an international cooperative project for development and testing of numerical models for the analysis of coupled thermal-hydrological-mechanical (THM) processes in geological media associated with nuclear waste isolation. The Swedish Nuclear Power Inspectorate (SKI) supports a collaborative research effort between Lawrence Berkeley National Laboratory (LBNL) and the Royal Institute of Technology (KTH) to actively participate in DECOVALEX, and to provide SKI with numerical models and model experiences on coupled THM processes. The work aims at strengthening SKI's capability to perform in-depth independent reviews of work conducted by the Swedish Nuclear Fuel and Waste Management Company (SKB) in the field of coupled THM processes. This is particularly important for analysis of Engineered Barrier Systems (EBS) and for the Performance Assessment (PA) of a future nuclear waste repository in the Swedish bedrock. This extended abstract describes the state of the art of coupled THM processes as a result of SKI's participation in the DECOVALEX project with particular emphasis on the relevance to the EBS.

SKI SUPPORTED NUMERICAL MODELS OF COUPLED THM ANALYSIS OF EBS SYSTEMS

As part of SKI's participation in the DECOVALEX project, two numerical tools have been developed, adapted and utilized by the LBNL/KTH for studies of coupled THM processes associated with nuclear waste repositories. The first one is ROCMAS, which is a finite element code for three-dimensional analysis of coupled THM processes of unsaturated/saturated porous and fractured geological media (Rutqvist et al. 2001a). The second code is TOUGH-FLAC, which has the capability of solving coupled THM problems under multiphase flow conditions (Rutqvist et al. 2002). These two codes complement each other; together they have the capability to analyze a large range of cases and scenarios related to coupled processes in EBS, both nearfield and far field of a future repository. The two codes are useful tools for performance assessment related to coupled THM processes at a future repository: The ROCMAS code can be used as the basic tool for the analysis of coupled THM processes and their impact on the stability and long-term performance of a repository. TOUGH-FLAC can be used for analysis of more specialized scenarios (e.g. degassing near waste canister, large strain fault slip, or long term creep). In comparing with codes ABAQUS and CODE_BRIGHT that are used by SKB's contractors, we conclude that ROCMAS and TOUGH-FLAC have sufficient capabilities to provide an independent check of SKB's work on coupled THM processes associated with the EBS.

TESTING AND APPLICATIONS WITHIN DECOVALEX PROJECT

Under various phases of DECOVALEX I, II and III, the following four major Test Cases (TC) have been studied related to EBS:

1. The BIG-BEN experiment at Tokai Works, Japan (Fujita et al. 1996).
2. The Kamaishi Mine heater test, Japan (Rutqvist et al 1999 and 2001b).
3. The FEBEX *in situ* experiment at the Grimsel Test Site, Switzerland (Rutqvist and Tsang 2004, Rutqvist et al. 2004a).
4. The Drift Scale Test at Yucca Mountain, Nevada (Rutqvist et al. 2004b and 2004c)

At the time of the BIG-BEN experiment, SKI did not have the independent model capability for analyzing coupled THM processes in unsaturated bentonite. Through continued participation in the DECOVALEX project and collaborative support of model development at LBNL/KTH, and SKI established the needed independent models and model experience for an independent analysis of coupled THM processes associated with EBS. SKI/LBNL/KTH has since been active in studying all the three latter Test Cases (TC) listed above and a number Bench Mark Tests (BMT). Note that these are three TCs (Kamaishi Mine, FEBEX and Yucca Mountain Drift Scale Test) are the most important large scale THM experiments internationally. In this report we shall describe the most recent efforts of particular relevance to the behavior of coupled THM on EBS and near-field problems: (a) FEBEX in situ experiment, and (b) a BMT that aimed at evaluating the importance of coupled THM processes in the nearfield of a KBS-3 type waste repository (Chijimatsu et al. 2004, Millard et al. 2004, Rutqvist et al 2004d). Participating in DECOVALEX has been very valuable, in that testing the models and has led to important improvements in adapting the models for analyzing coupled THM processes associated with nuclear waste repositories.

STATE OF THE ART AND LESSONS LEARNED

The work within the DECOVALEX project including simulation of the above-mentioned *in situ* experiments and a number of BMTs have shown that most coupled THM processes can be predicted with confidence through rigorous and carefully executed numerical modeling, based on a sufficiently accurate material characterization and model conceptualization. In general, temperature, fluid pressure, and saturation can be most accurately predicted, while the mechanical and hydromechanical behavior of the fractured rock mass and bentonite are more complex and difficult to predict. The analysis shows that it is not possible to predict mechanical and hydromechanical responses at every point of a fractured rock mass. The presence of fractures implies that there is substantial spatial variation in the responses of (for example) fluid flow and displacements. Therefore, it might only be possible to predict hydromechanical changes (e.g., mechanically induced changes in permeability) in a statistical sense. It is concluded that prediction of hydromechanical responses in fracture rock surrounding a repository should therefore include a stochastic approach considering heterogeneity, not only on hydraulic properties, but also on mechanical and hydromechanical properties. It has been confirmed that fully coupled THM modeling is necessary for the performance of a multiple-barrier nuclear waste repository. A coupled THM analysis is absolutely essential for the analysis of mechanical behavior in both the buffer and surrounding rock mass. This importance of various couplings for the EBS and surrounding fractured rock is illustrated in Figure 1, where the most important couplings to be considered is emphasized with a thick arrow.

OUTSTANDING ISSUES

The DECOVALEX project has also helped to reveal some outstanding issues related to predicting coupled THM processes in the EBS and surrounding fractured rock. Through SKI/LBNL's work in DECOVALEX III it has been shown that rate of buffer resaturation and fluid pressure restoration processes might be very important for the stability of the rock walls of deposition holes. Simulation within the recent DEOCALEX III project, indicates that a delay in the resaturation and fluid-pressure restoration in the buffer may jeopardize the mechanical stability of excavation walls after closure of the repository. This was shown in a sensitivity study involving a KBS-3 type of multiple-barrier nuclear waste repository where two cases of timely or delayed resaturation of the buffer and back-fill were simulated. A delayed resaturation of the buffer were obtained when the deposition hole was located in an unfractured low permeability rock as shown in Figure 2. The delayed resaturation of the buffer resulted in a delayed development of compressive stress in the buffer and back-fill. As a consequent, the back-fill will not provide sufficient support stress to the rock walls, which then are prone to failure. If, on the other hand, the resaturation of the buffer and back-fill occurs timely (within tens of years rather than hundreds of years), compressive stress will develop within the buffer and back-fill in time to provided sufficient support before thermal rock stresses are fully developed. A fully developed support stress on the rock wall will tend to prevent rock mass failure as shown in Figure 3. However, several *in situ* tests (e.g., Kamaishi Mine heater test and FEBEX) indicates that the resaturation of the buffer may be delayed because of bentonite's microstructural changes under HM processes. Such delay in resaturation of the buffer may be detrimental to the stability of the surrounding rock walls, which then will experience much more mechanical changes over the course of the thermal post-closure cycle.

CONCLUDING REMARKS AND RECOMMENDATIONS

With the experience in participating in the DECOVALEX project SKI/LBNL/KTH are in a position to independently examinate of SKB's work related to EBS and coupled THM processes. The two SKI supported numerical models ROCMAS and TOUGH-FLAC have the same capabilities as SKB's numerical models, and in certain aspects exceed the capabilities of SKB's numerical models. This is important, because SKI needs not only to investigate what SKB does but also what they are not doing, thus providing them with guidelines and insightful comments. Maybe the most important gain of the DECOVALEX project is the experience in solving realistic problems related to EBS and coupled THM processes, which provide experiences and depth of knowledge needed for assessing future analyses of a real site. This is extremely valuable, because the most important asset is not the numerical model (provided that it meets certain requirements), but the knowledge of how to adapt and apply numerical models correctly for specific problems.

The next phase of the DECOVALEX project (DECOVALEX-THMC) will be extended from coupled THM to coupled THMC processes, where C stands of chemical processes. This will include several bench mark studies of coupled THMC processes within the bentonite buffer as well as at the excavation disturbed zone near the interface between bentonite and rock. Coupled THMC modeling will be carried out by sequential coupling of TOUGH-FLAC to TOUGH-REACT, which is an LBNL code for reactive transport analysis. The processes studied in DECOVALEX-THMC may include long term degradation of bentonite and rock and its consequences on long term integrity of a repository. In addition, further work on the consequences of potentially delayed resaturation of buffer and back-fill as a result of the microstuctural behavior is recommended.

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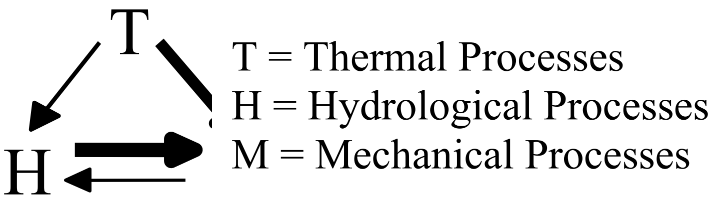
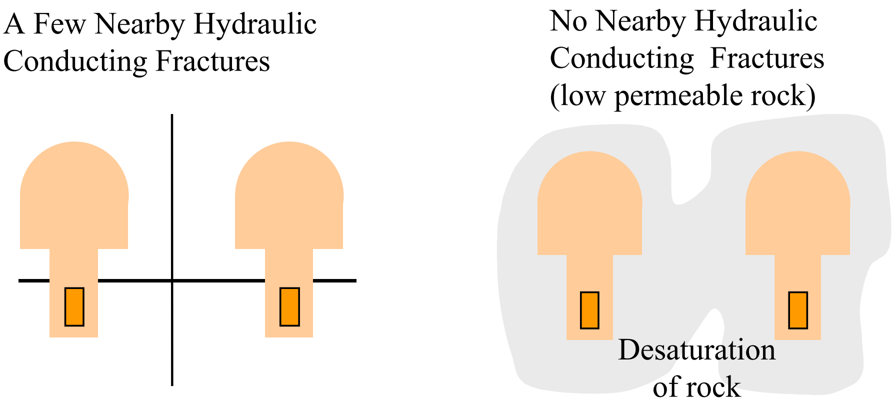


Figure 1. The importance of various THM coupling is illustrated by the thickness of the arrows, with thickest arrow signifying the most important coupling to be considered.

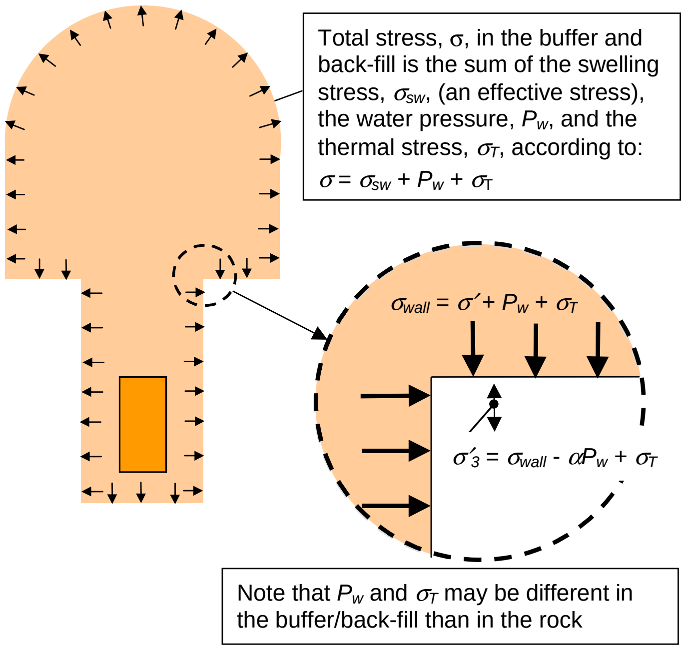

A Few Nearby Hydraulic Conducting Fractures

No Nearby Hydraulic Conducting Fractures (low permeable rock)

- Sufficient water provided to buffer to avoid desaturation of surrounding rock
- Timely saturation and swelling of buffer and back-fill
- Timely restoration of fluid pressure and compressive stress within buffer and back-fill

- Suction from bentonite induces desaturation of surrounding rock
- Delayed saturation and swelling of buffer and back-fill
- Delayed restoration of fluid pressure and compressive stress within buffer and back-fill

Figure 2. Comparison of simulation results for timely and delayed resaturation of buffer and back-fill.



Total stress, σ, in the buffer and back-fill is the sum of the swelling stress, σ_{sw}, (an effective stress), the water pressure, P_w, and the thermal stress, σ_T, according to:

$\sigma = \sigma_{sw} + P_w + \sigma_T$

Note that P_w and σ_T may be different in the buffer/back-fill than in the rock

Figure 3. Illustrates how a fully developed compressive stress in the buffer and back-fill provides support stress to the rock wall which are then prevented from failure.

The Effects of High Salinity Groundwater on the Performance of Clay Barriers

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Background

Potential changes in groundwater chemistry during the operational or post-closure periods of the Swedish repository for spent fuel could affect the performance of both the bentonite buffer and repository backfill. For example, the introduction of dilute groundwaters during drawdown could increase the potential for bentonite erosion and/or the production of colloids. Alternatively, the up-coning of saline groundwater could lead to decreased swelling pressures in both the bentonite buffer and tunnel backfills, and could also induce ‘piping’[4]. SKB is considering these issues as part of its ‘SR-Can’ safety assessment (SKB, 2004a, b, c). *Inter alia*, they have derived ‘function indicators’ for the hydraulic conductivities and clay swelling pressures in the buffer and backfill with regard to groundwater salinity as shown in Table 1.

SKB concludes that if the buffer density exceeds 1.9 Mg m^{-3}, the functional requirements for the swelling pressure to exceed 1 MPa will be fulfilled, even with groundwater salinities equivalent to 3 M NaCl (SKB, 2004a) [Figure 1]. Similarly, the functional requirement for buffer hydraulic conductivity of 10^{-12} m s^{-1} will also be fulfilled if the buffer density is greater than 1.8 Mg m^{-3}, even for 3M NaCl equivalent salinity (SKB, 2004a) [not illustrated here]. SKB also concludes that the swelling pressure criterion is likely to be met for a MX-80 bentonite/crushed rock backfill of 1.7 Mg m^{-3} mixed dry density at low salinities, but not for a backfill employing Milos bentonite (SKB, 2004a). The hydraulic conductivity functional criterion is likely to be met for both backfill types at all salinities (SKB, 2004a).

Currently, SKB envisages the presence of two water types at its repository sites: fresh waters with a bicarbonate imprint at less than 200 m depth; and brackish-marine waters with Cl^- contents up to 6 g/l (10 g/l TDS) [SKB, 2004a]. The most saline groundwater being considered by SKB in any up-coning process has 47.2 g/l TDS and is exemplified by a water from the Laxemar borehole at 1350 m depth (SKB, 2004a).

The ‘buffer rheology model’ is described in SKB (2004a) and in more detail in Hedin (2004) and relies upon the calculation of buffer density assuming that upward expansion of the buffer is balanced by friction against the walls of the deposition hole and the force exerted by the compressed tunnel backfill. This sub-model can handle the

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[4] ‘Piping’ refers to the erosion of material (clay) along a linear feature due to instability in response to water pressure. Piping takes place if the water pressure in a fracture in the deposition hole is higher than the counteracting pressure from the clay and its shear resistance. Increased salinity of groundwater increases the likelihood of piping (SKB, 2004b).

interaction with saline groundwater through consideration of the osmotic effects described by Karnland et al. (2002).

Table 1 Function indicators for the bentonite buffer and backfill. From SKB (2004a).

	Criterion	**Rationale**
Buffer		
Hydraulic conductivity	$< 10^{-12}$ m s^{-1}	avoid advective transport
Swelling pressure	> 1 MPa	ensure tightness, self-sealing
Groundwater salinity	[NaCl] < 100 g/l	avoid detrimental effects on swelling
Backfill		
Hydraulic conductivity	$< 10^{-10}$ m s^{-1}	limit advective transport
Swelling pressure	> 0.1 MPa	limit buffer expansion
Groundwater salinity	[NaCl] < 35 g/l	avoid detrimental effects on swelling

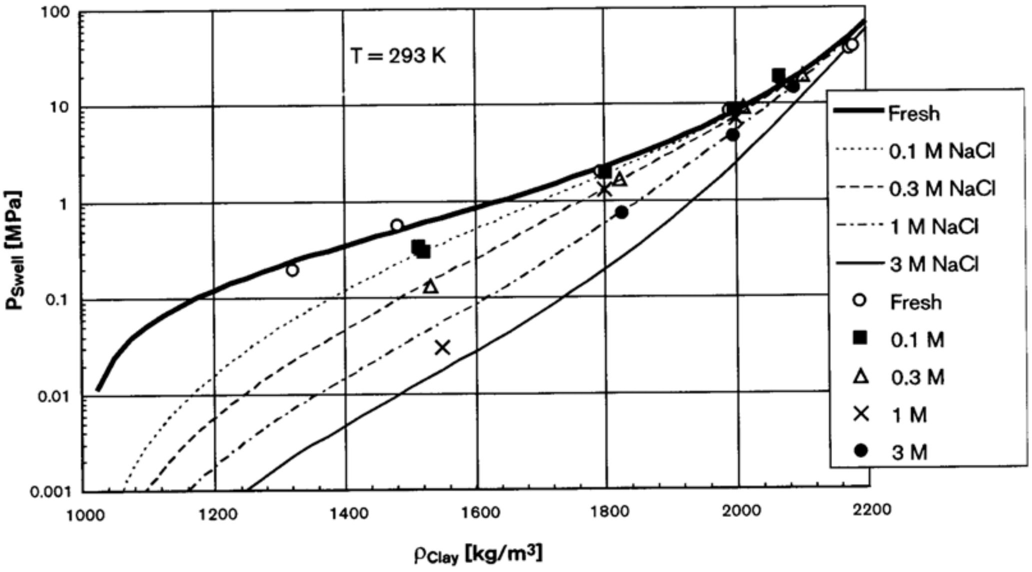

Figure 1 Comparison of experimentally-determined and modelled values of swelling pressure for different densities of MX-80 bentonite at different pore fluid salinities. From Hedin (2004).

Treatment of clay swelling behaviour in SR-Can

SKB consider that the swelling pressure of the buffer under fully-saturated conditions is a function of the cation exchange capacity of the clay, the clay density, and the ionic composition of the surrounding groundwater (Hedin, 2004). According to Hedin (2004), the relationship between swelling pressure and clay density for freshwater is:

$$P_s^{fresh} = AT\left(\exp\left(B\frac{\rho_{solid}\left(\rho_{clay} - \rho_{water}\right)}{\rho_{water}\left(\rho_{solid} - \rho_{clay}\right)}\right) - 1\right) \qquad (1)$$

where A and B are fitting parameters, T is temperature (°K), and ρ_{clay}, ρ_{water}, and ρ_{solid} are the densities of saturated clay, water, and solid clay particles, respectively.

For saline groundwater, Hedin (2004) considers that the swelling pressure will be reduced due to osmotic effects, leading to a 'Donnan equilibrium'. This loss of pressure is confirmed by results from laboratory experiments (Karnland, 1997). Hedin (2004) deduces the following relationship for the clay swelling pressure in an external NaCl concentration C [M] where Na^+ is the adsorbed cation on the clay:

$$P_s^{saline} = \sqrt{\left(P_s^{fresh}\right)^2 + \left(2RTC\alpha_d\right)^2} - 2RTC\alpha_d \qquad (2)$$

where P_s is the swelling pressure in kPa, R is the gas constant [8.314 J/(°K.mole)] and α_d (dimensionless) is the tabulated degree of dissociation for the external NaCl solution of concentration C, given by:

$$\alpha_d \approx 10^{\frac{-0.34\sqrt{C}}{1+1.83\sqrt{C}}} + 0.03C \qquad (3)$$

Fundamental clay behaviour

Smectite clays can absorb water into clay inter-layers with the most important parameters being:

- the surface density of charge of the clay;
- the charge and solvation behaviour of the inter-layer ions;
- and the electrolyte concentration or activity of water.

Two categories of swelling are generally observed in clays (Madsen and Müller-VonMoos, 1989):

- *innercrystalline swelling* caused by the hydration of the exchangeable cations in the dry clay;

- and *osmotic swelling* resulting from concentration gradients in ion concentrations between clay surfaces and pore water.

Madsen and Müller-VonMoos (1989) describe the clay swelling process in montmorillonite. According to them, innercrystalline swelling may result in a doubling of clay volume and is generally stepwise (Figure 2). Emplacement of the first water layer leads to a layer widening of 0.25 nm. The cations are partly coordinated by the oxygen of the siloxane surface. With two water layers, the interlayer cations are coordinated octahedrally. With further water uptake, the coordinated octahedron alters its orientation. This stepwise nature of the layer widening process may be examined using water vapour adsorption isotherms (Figure 3).

The swelling pressure due to *innercrystalline swelling* can be calculated from the water vapour adsorption isotherms. In sodium montmorillonite, the sodium ions move to the layer surfaces as more water is taken up. Electrical double layers are built up which ultimately lead to disintegration of the montmorillonite into individual layers. Calcium montmorillonite behaves very differently from the sodium variety, in that swelling generally ceases once the distance between clay layers reaches about 1 nm. The calcium ions remain on the plane halfway between neighbouring layers and continue to exert an electrostatic attraction between them. Double layers are only formed on the outer surfaces of Ca-montmorillonite particles.

Osmotic swelling operates over larger distances than innercrystalline swelling and in sodium montmorillonite can result in total separation of clay layers. Because the interlayer ions are fixed for electrostatic reasons, water is taken up into the interlayer spaces to balance concentration, provided there is a higher concentration in the interlayer spaces. Osmotic swelling depends to a large extent on the electrolyte concentration and the valency of the dissolved ions. Innercrystalline swelling, on the other hand, depends only slightly on these factors. However, the swelling pressures are much smaller than innercrystalline swelling and barely exceed 2 MPa. The driving force for osmotic swelling is the large difference in concentration between the ions held electrostatically to the clay surface and the ions in the pore water of the clay (Figure 4). The negatively charged clay surface and the cloud of ions form the diffuse electrostatic double layer. Increasing the salinity of the pore water removes water from between the clay layers and decreases the swelling pressure. Similarly, conversion of the Na-montmorillonite to the Ca-form reduces the swelling pressure.

Several models are available for the prediction of swelling pressure in montmorillonite-type clays and these are reviewed in Grauer (1986) and Karnland (1997). Essentially, the models are of three types:

- empirical models.
- Diffuse double-layer models.
- Thermodynamic models.

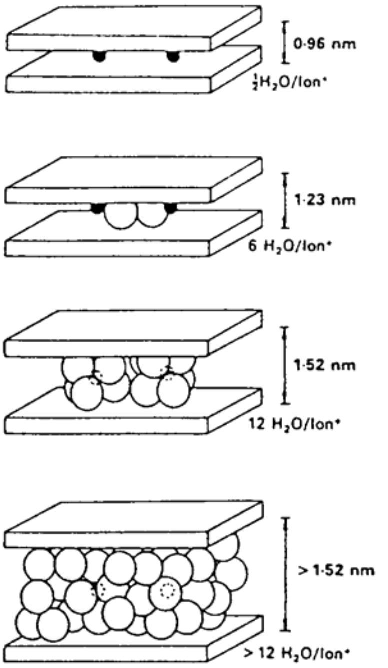

Figure 2 Innercrystalline swelling of sodium montmorillonite showing the change of interlayer distances with stepwise increases in the number of water molecules. From Madsen and Müller-VonMoos (1989).

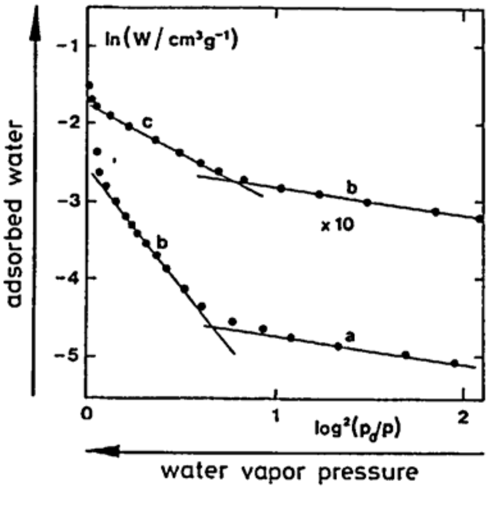

Figure 3 Water vapour adsorption isotherm for Wyoming bentonite at 20 °C. Sections b and c correspond to the interaction of the first and second water layers, respectively. The values on the top curve have been magnified ten times. W = water content, p = relative water vapour pressure at saturation. From Madsen and Müller-VonMoos (1989).

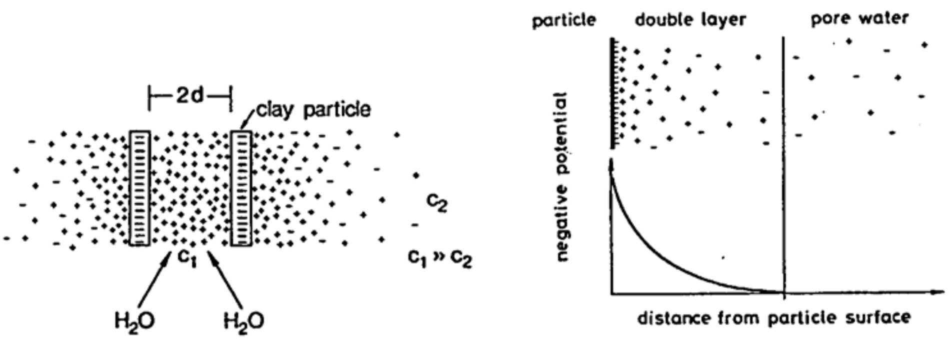

Figure 4 Two negatively charged clay layers with ion cloud and illustration of the diffuse double layer and ions in the pore water. The ion concentration C_1 between the layers is much higher than the ion concentration C_2 in the pore water. Equilibration of the concentrations can only be achieved though the penetration of water into the space between clay layers since the interlayer cations are fixed electrostatically by the negative charge of the layers (osmotic swelling). From Madsen and Müller-VonMoos (1989).

Empirical models are attractive because of their simplicity, but data fitting sometimes necessitates the use of negative values for clay interlamellar distances, thus questioning the physical significance of the models (Karnland, 1997).

Double layer models use the eponymous model developed by Gouy and Chapman in 1910 and account for both the repelling forces between clay particles and attractive van der Waals forces. Komine and Ogata (1986) have used the diffuse double layer theory to calculate swelling pressures in bentonite clays and considered that the model predicts pressures well up to 3 MPa. However, Karnland (1997) applied their model to MX-80 bentonite in solutions of variable NaCl content and noted that the capacity of the model to predict swelling pressures in saline solutions with NaCl > 0.5 % was very limited. Yong (1975) used an osmotic diffuse double layer model to calculate bentonite swelling pressures by means of the Van't Hoff equation. Calculations of swelling pressure using this model fit measured values reasonably well up to pressures of 30 MPa, but at high salt concentrations, the measured pressures exceed calculated values (Karnland, 1997). In general, double layer models involve inconsistencies in their mathematical treatment and there are issues concerning parameterisation of the models (Karnland, 1997).

Thermodynamic models describe the macroscopic properties of the clay-water system and do not lend themselves to consideration of microscopic properties (Sposito, 1972). In general, thermodynamic models consider the vapour pressure of clay-water systems (Low, 1987):

$$P_s = -\frac{RT}{M.\bar{v}_w}\ln\left(\frac{p}{p_0}\right) - \left(-\frac{RT}{M.\bar{v}_w}\ln\left(\frac{p_e}{p_0}\right)\right) \qquad (4)$$

where M is the molecular weight of water, $\bar{v}_w$ is the partial specific volume of water, p is the vapour pressure of adsorbed water, p_0 is the vapour pressure of pure water, and p_e is the vapour pressure of the surrounding electrolyte solution. The first term in equation (4) represents the swelling pressure of the clay and the second term addresses the osmotic pressure of the surrounding salt solution.

The use of equation (4) to calculate the swelling pressure of MX-80 bentonite in saline solutions would suggest a zero pressure in a 1.25M NaCl solution, but unfortunately, this is not borne out by experimental results (Karnland, 1997). Karnland (1997) has suggested modification of equation (4) to account for a change in the partial molar free energy of water in the clay-water system:

$$P_s = -\frac{RT}{M.\bar{v}_w}\ln\frac{p}{p_0} + \left(-\frac{RT}{M.\bar{v}_w}\ln\frac{p_{ie}}{p_0}\right) - \left(-\frac{RT}{M.\bar{v}_w}\ln\frac{p_e}{p_0}\right) \tag{5}$$

where p is the vapour pressure in the clay-water solution as saturated by pure water and p_{ie} is the vapour pressure in a water solution as saturated by the electrolyte solution.

SKB currently prefer an interpretation of clay swelling pressure involving so-called ‘Donnan exclusion’ where clay particles are considered as macro-ions and the entire clay-water system may be viewed as a polyelectrolyte. Swelling pressures are calculated using a Van’t Hoff expression [equation (1)] which simulates measured swelling pressure in saline solutions much more accurately than previous models (Karnland, 1997).

Dixon (2000) considers that the debate concerning the validity of the various theoretical models describing clay swelling pressure is unlikely to be settled in the near future and suggests that effort may be best placed in the acquisition of a database of physical measurements. A compilation of bentonite swelling pressure data produced by Dixon (2000) suggests little distinction of swelling pressures with regard to groundwater salinity (Figure 5). These data would suggest that a clay density of 0.9 Mg m^{-3} would be sufficient to produce a swelling pressure of 0.1 MPa at any groundwater salinity.

There has been extensive work carried out in Germany regarding the performance of bentonite in highly saline solutions as a result of their potential use as seals in halite repository host rocks (Herbert and Moog, 2001). The precise composition of brines has been shown to affect bentonite swelling pressures. For example, the presence of Mg increases swelling pressure due to its large hydration sphere, whereas K produces a decrease. The authors suggest that the knowledge of the swelling pressure of bentonite in highly saline solutions is currently insufficient for use in predictive modelling. Factors such as dry density, microstructure, sample flooding regime and sample dimensions seem to have a bigger influence on swelling pressure in laboratory experiments than brine composition. GRS plan to acquire more data to develop predictive models further.

Another conclusion from these studies is that bentonite is not stable in the long-term in brines (Herbert and Moog, 2001; Hofmann et al., 2004).

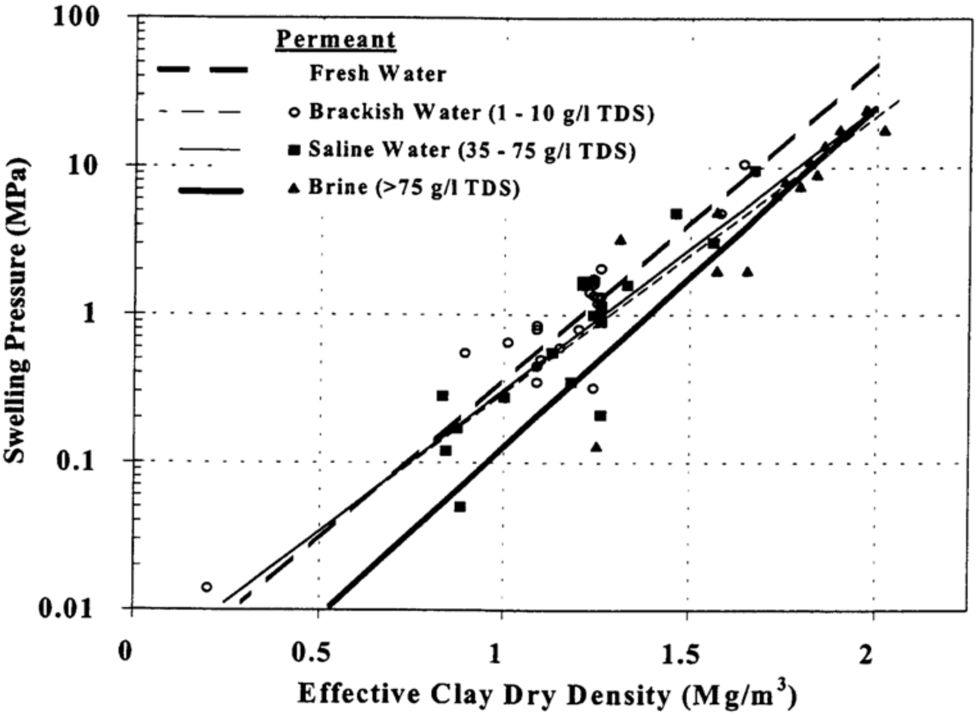

Figure 5 Relationship between bentonite swelling pressure and groundwater salinity. From Dixon (2000).

Repository Backfilling

The issue of clay swelling behaviour is also of relevance to repository backfilling. SKB (Gunnarsson et al., 2004) state the following requirements for repository backfill:

- compressibility: the backfill should have a low compressibility to maximise the density of the buffer by limiting any upward expansion of the latter.
- hydraulic conductivity: the backfill should have a hydraulic conductivity over the entire length and cross-section of a tunnel in the same order of magnitude as that of the surrounding rock.
- effects on other barriers: the backfill should have no negative influences.
- long-term stability: the backfill should be stable and its functions maintained in the long-term.

SKB is currently studying different designs for tunnel and repository backfilling (Gunnarsssson et al., 2004). With regard to salinity effects, they state that a hydraulic conductivity of 10^{-10} m s^{-1} and a swelling pressure > 0.1 MPa at a groundwater TDS of 35 g/l is the target for this assessment.

SKB considered 5 backfill types in their review:

A. bentonite and crushed rock in various proportions (from 15 to 30 wt% bentonite) applied in inclined layers (e.g. Börgesson et al., 1997).
B. Compaction of swelling Friedton Clay, applied in a manner similar to concept A.
C. Compaction of non-swelling soil (glacial till) with bentonite blocks at roof level.
D. Pre-compacted blocks of bentonite across the entire tunnel section.
E. A 'sandwich concept' of alternating zones of bentonite above the disposal holes and crushed rock elsewhere.
F. A 'compartment concept' of alternating zones of bentonite and crushed rock, with the difference with the sandwich concept being the length of the crushed rock zone (constant in the sandwich concept and varying in the compartment concept according to local geology and hydrogeology).

From this review, SKB consider that concepts A, B, and D should receive further attention in Phase 2 of their joint studies with Posiva.

Dixon (2000) considers that the backfill is much more sensitive to variations in groundwater salinity than the bentonite buffer due to the lower clay content of the former and suggests an initial density of at least 0.9 Mg m^{-3} to maintain a nominal swelling pressure of 0.1 MPa.

Piping

SKB (2004b) states that if groundwater inflow in fractures in deposition holes exceeds that which can be absorbed by bentonite swelling, there will be a water pressure in the fracture acting on the buffer. Since the bentonite is initially in a gel-like state, the gel may be too soft to stop the water inflow and piping may result. Piping is the erosion of the clay along a linear feature. SKB (2004b) goes onto state that piping will take place if the following conditions are fulfilled:

- The water pressure in the fracture must be higher than the total pressure in the clay and the clay's shear resistance.
- The hydraulic conductivity of the clay must be so low that water flow into the clay ceases to counteract the water pressure in the fracture.

SKB believe that piping will only occur before full saturation of the buffer. SKB view *erosion* as a different process which takes place if drag forces on clay particles from water movement is higher than the sum of frictional and attractional forces between the particle and the clay structure (SKB, 2004b). Erosion could occur as a consequence of piping, but also in the long-term at the interface between water-bearing fractures and the bentonite. Erosion will therefore concern clay gel which has penetrated these fractures during swelling.

Clearly, for buffer functions to be maintained in the long-term, it is essential that buffer swelling closes any channel opened by piping. This will be the case if mass transfer by buffer swelling is greater than the erosion/piping rate and that piping does not re-occur (SKB, 2004b).

Piping is especially relevant to the horizontal emplacement concept where channels may contact a large number of canisters. This is currently being investigated by SKB (SKB, 2004b). More information may also be gained from excavation of the Prototype Repository test at Äspö (in 10 years time) where one of the deposition holes has a relatively large water inflow. SKB will investigate piping effects in SR-Can during the pre-saturation phase and will be based mainly on experience from the KBS-3H study (SKB, 2004b).

The problem of piping is also germane to repository backfilling. SKB consider that it may be difficult to derive a solution to water inflow during backfill installation and thus: *"piping can probably not be avoided in the installation phase, irrespective what type (sic) of backfill material is used"* (Gunnarsson et al., 2004). Gunnarsson et al. (2004) consider that a point source of groundwater inflow as low as 1 l/min would probably result in piping and surface erosion of the tunnel backfill. Consequently, the backfill needs to have enough swelling ability so that piping channels can be healed once a tunnel has been sealed by plugging. All this must be placed in context of the rate of backfilling which SKB hopes to be in the order of 6 m per day.

Conclusions

Available experimental data demonstrate that high salinity groundwaters will decrease clay swelling pressures in the bentonite buffer and backfill. Interpretation of these data is not unequivocal and further research is required to develop more consistent predictive models. Further experimental data would also improve statistical interpretations. It is noteworthy that GRS in Germany are interested in this issue and have embarked on a programme of data acquisition.

The groundwater salinity issue is irrelevant if emplaced buffer/backfill density can be guaranteed. Buffer and backfill densities of 1.9 and 1.7 Mg m^{-3}, respectively would ensure adequate swelling pressure (> 1 and > 0.1 MPa, respectively) and hydraulic conductivity ($< 10^{-12}$ and $< 10^{-10}$ m s^{-1}, respectively), regardless of groundwater salinity. However, achievement of the requisite buffer density is critically dependent upon compensation for annular voidage between the compressed bentonite rings and the copper canister and the deposition hole rock walls upon buffer emplacement (SKB, 2004a).

Achievement of the requisite backfill density will depend upon the final adopted formulation and emplacement methodology (currently undecided). Emplacement of bentonite/rock backfill (30:70) in the Backfill and Plug test at Äspö HRL achieved a mean density of 1.65-1.7 Mg m^{-3} (Gunnarsson et al., 2001).

Piping is an issue for both bentonite buffer and backfill and may be unavoidable for localised high groundwater inflows. SKB need to demonstrate how they will address this problem in SR-Can and in any future assessments.

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EC Activities on Geological Disposal of Radioactive Wastes

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Euratom of EC began work on geological disposal in 1975. The EC shares the costs of work with EU Member States and organizes work in programs that normally last about five years. The earliest work focused on identifying potentially suitable geological formations in Europe. Since 1979, work has effectively fallen into two main categories: scientific and technical studies on the long-term safety of disposal and experimental and engineering work that is carried out in underground laboratories, such as the Äspö Hard Rock Laboratory and the Mol facility in clay in Belgium. Through agreements with non-EU countries, work has also been carried out in other underground facilities, e.g. in Canada and the USA.

Working together in EC programs has given added value to solving the waste problem by bringing together a large number of academic and professional scientists from waste disposal implementers and regulatory agencies which has resulted in wide and efficient dissemination of results to the end users. The two most recent research and development programs (Fourth and Fifth Framework Programmes: 1994 – 2002) saw the evolution of co-ordination of national activities, which had driven earlier programs. Today, as the geological disposal concept moves to implementation, the emphasis is much more on integration of efforts in order to rationalize and optimize solutions that can be achieved in Europe. In the following sections the principal achievements of the FP 5 is presented.

Achievements of FP 5

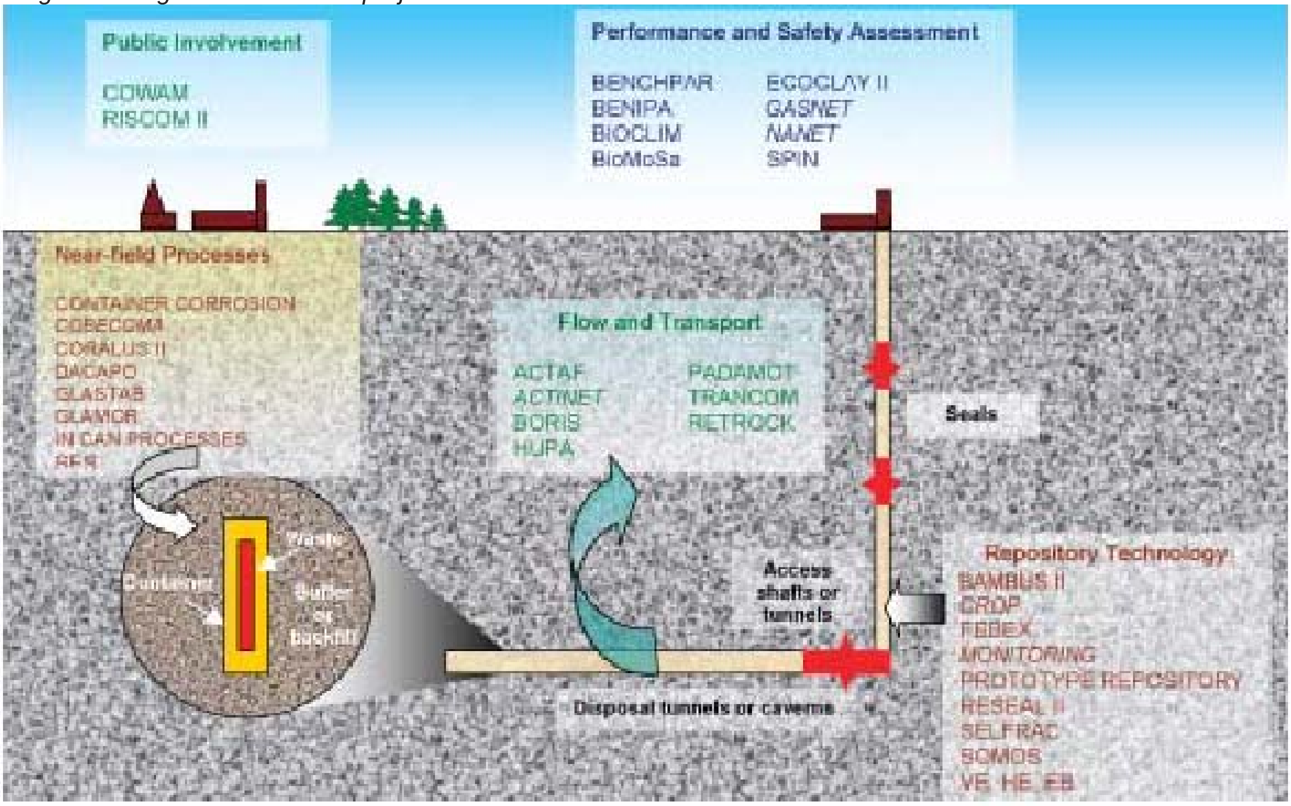
The main achievements of the Fifth Frameworke Programme 1998 – 2002 can be described under the following thematic headings:

- Development of repository technology
- Long-term behavior of wastes, containers, buffer and backfill
- Groundwater and radionuclide movement around repositories
- Safety assessment of geological disposal
- Public Involvement in repository programs

Of particular interest to this workshop is the content in the second bullet dealing with the long-term behavior of wastes, containers, buffer and backfill and in particular the buffer and backfill.

The 5th Framework Programme was supporting 43 projects in the 'Radioactive Waste Management' priority area, from which 25% are Thematic Networks (TN) and Concerted Actions (CA), and had an EC financial contribution of about 29 M€. The projects and their belonging to the thematic headings listed above are depicted in the integration diagram below.

Integration diagram of FP5 RTD projects and Thematic Networks



Most of the projects listed under Near-field Processes deal with properties and behavior of the waste material.

Repository technology

Projects related to buffer and backfill are mostly listed under Repository Technology in the figure above. They are and deal with the following:

- EB & VB – Engineer barrier emplacement and ventilation experiments at Mt Terri
- FEBEX - Full-scale engineered barriers experiment in crystalline rock – phase II
- PROTOTYPE REPOSITORY – Full-scale testing of the KBS-3 concept for HLW
- SELFRAC – Fractures and self-healing within the EDZ in clays

EB & VB – Engineer barrier emplacement and ventilation experiments at Mt Terri

The EB experiment aims to demonstrate a new concept for the construction of HLW repositories in horizontal drifts, in competent clay formations. The principle of the new construction method is based on the combined use of a lower bed made from compacted bentonite blocks, and an upper backfill made with a bentonite-pellets-based material. After emplacement testing in a 6 m long, 3 m in diameter tunnel model, of different methods (pneumatic, auger, belt conveyor), it has been demonstrated that auger method provides the highest emplaced dry density without major gaps.

The VE experiment is a ventilation test carried out *in situ* in a 1.3 m diameter by 10 m long horizontal tunnel. The objectives of the test were to estimate the desaturation and resaturation times in clay rock, produced by drift ventilation; the saturated hydraulic conductivity of the rock (macro-scale) and comparison with values obtained at smaller scales and evaluation of the scale effect impacting this important parameter; and the evolution of the EDZ, in terms of changes in hydraulic conductivity and of displacements caused by the generation of cracks on drying.

FEBEX - Full-scale engineered barriers experiment in crystalline rock – phase

The overall aim of the project is to study the behaviour of the engineered barrier components of a high-level radioactive waste repository in granite. The project has so far comprised two phases which include an in-situ test at the Grimsel underground laboratory (Switzerland), a mock-up test (for controlled conditions) above ground in Spain, and a series of laboratory tests and numerical modelling of all the tests. The FEBEX II work is to improve knowledge of the THM and THMC processes, especially in a more hydrated clay barrier, in order to improve, calibrate and validate existing numerical codes. The major achievements of the project so far have been:

- The feasibility of constructing engineered barriers for the horizontal storage of canisters placed in drifts has been demonstrated. Specifically, it has been shown that the manufacturing and handling of bentonite blocks is feasible at industrial scale and that the clay barrier may be constructed with a specified average dry density in order to achieve the permeability and swelling pressure required for the barrier.
- The CODE-BRIGHT numerical THM model is capable of reasonably predicting the measured results of the two large-scale tests. During this period, it has been necessary to modify justminor details of the model as it has been observed that its core is based on solid physical laws.

PROTOTYPE REPOSITORY – Full-scale testing of the KBS-3 concept for HLW

The main objectives of the project are to use engineering, full-scale demonstration and *in-situ* testing to prove the feasibility of a repository concept for hard rock, using the Äspö hard rock laboratory in Sweden. The prototype repository consists of two tunnel sections with four and two canister deposition holes respectively. The outer section should be dismantled after five years of operation, while the other section may be operated for up to 20 years. A tunnel-boring machine (TBM) with diameters of 5 m for the tunnel and 1.75 m for the vertical holes was used for excavation. The boring of the horizontal drift was based on proven technology, while the vertical boring needed more accurate precisions than ever done before.

The project used “MX-80” bentonite from Wyoming for the buffer. Techniques have been developed, following co-operation between Spain and Sweden, for the compaction of blocks with dimensions ranging from brick size to cylinders with a diameter of 1.65 m and height of 0.5 m.

SELFRAC – Fractures and self-healing within the EDZ in clays

The main objectives of the project are to characterize the Excavation Damaged or Disturbed Zone (EDZ) in clay and its evolution with time, as it may lead either to a significant increase in permeability related to diffuse and/or localized crack proliferation, or (as a result of self-sealing and self-healing) a reduction in permeability with time. Two potential geological formations for deep radioactive waste repositories were studied: the Opalinus clay (Switzerland) and the Boom clay (Belgium). During selfsealing the permeability decreases up to values close to the permeability of intact Boom clay (about 4.10-12 m/s).

Safety and performance assessment

In FP5 all aspects of the behavior of bentonite at a process model level and how its properties are translated into PAs were studied. Process models that describe materials behaviour in a repository need to consider all of the driving mechanisms – thermal, chemical, hydraulic and mechanical ('TCHM') resulting from the radioactive decay heating of the wastes, the chemical composition of materials and pore waters, and the rock stresses. These can each be affected by external events, too – for example, in the distant future, by glaciation cycles. The following projects had a strong component of bentonite studies in them:

- BENIPA – Bentonite barriers in integrated performance assessment
- BENCHPAR – Benchmark tests and guidance on coupled processes for performance assessment of nuclear waste repositories
- ECOCLAY II – Effect of cement on clay barrier performance

BENIPA – Bentonite barriers in integrated performance assessment

An in-depth analysis and cross comparison has been made of the different models available for the numerical simulation of the behaviour of bentonite barriers at different levels of detail. The consistency and availability of data needed by the models has been evaluated. The overall result is a better understanding of the modelling and computer programs related to the performance of bentonite barriers.

BENCHPAR – Benchmark tests and guidance on coupled processes for performance assessment of nuclear waste repositories

This project was conducted as a part of the international DECOVALEX project. In the near-field rock-buffer system, a series of THM analysis was performed on homogeneous and fractured rock masses. The importance of the couplings on the safety indicators was evaluated by comparing the THM calculations to partially coupled ones (e.g. TM, TH, HM). Coupling is most important in the short term (less than 100 years) and it has been concluded that for confidence building and demonstration purposes, a fully coupled approach is necessary.

ECOCLAY II – Effect of cement on clay barrier performance

This project dealt with the understanding of the physico-chemical behavior of argillaceous and granitic rocks altered by the effect of a hyperalkaline plume. Data was acquired on sorption and migration of radionuclides, on mineralogical transformations and modifications to the properties of bentonite, of clay and crystalline host rocks in contact with either alkaline fluids or different kinds of cement.

The Sixth Framework program FP6 (2002-2006)

The overall theme of FP6 is the sustainable integration of European research in the geological disposal of radioactive waste and to identify and answer outstanding questions. The programme is more focused, more integrated, with fewer larger projects, and involving more partners.

Available information about the content of project results in FP5

The information presented in this abstract is received from the EC General Information: “Geological Disposal of Radioactive Wastes Produced by Nuclear Power .. from concept to implementation”
ftp://ftp.cordis.lu/pub/fp6-euratom/docs/waste_disposal_eur-21224_en.pdf

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