SKI Report 2003:29

Research

# Long-term Integrity of the KBS-3 Engineered Barrier System

Report from Workshop at Krägga Herrgård, Bålsta, Sweden,
6-8 November 2002

**Synthesis and Extended Abstracts**

Swedish Nuclear Power Inspectorate
August 2003

ISSN 1104–1374
ISRN SKI-R-03/29-SE

# Foreword

As part of preparations for review of future license applications, the Swedish Nuclear Power Inspectorate (SKI) organised a workshop on engineered barrier integrity of the KBS-3 concept, held 6-8 November 2002. The main topic of the workshop was the combined consideration of the copper canister and bentonite buffer, as well as the assessment of both chemical and mechanical aspects of engineered barrier integrity. The reason for addressing these topics was to identify critical issues related to engineered barrier performance, which has to be dealt with in greater detail during the coming few years. The workshop included presentations related to engineered barrier integrity by external experts, and working group sessions. The latter focussed on three time scales; the fabrication and pre-closure period, the initial thermal period and the long-term isolation period. This report includes a synthesis of the working group discussions and extended abstracts for the presentations. The conclusions and viewpoints presented in this report are those of one or several workshop participants. They do not necessarily coincide with those of SKI.

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# 1. Introduction

The long-term safety of a future spent-fuel repository in Sweden relies on the long-term isolation (> 100 000 years) that is provided by the copper canister embedded within a low-permeability clay barrier (SKBF 1983, SKB 1999). This can be regarded as the most basic safety function for the KBS-3 design concept. However, in performance assessment (PA), considerable attention also has to be devoted to other safety features such as slow radionuclide release and subsequent retardation provided by the engineered barrier system (EBS) and the geosphere. This is to demonstrate that safety does not depend on any one particular isolation function.

In the evaluation of the various mechanisms that could compromise the canister integrity, it is important to acknowledge that the bentonite-clay buffer serves a key role in physically protecting the copper canister, and that the properties of the near-field rock in turn affect the buffer. It is therefore essential to integrate the analysis of the functions of these three components, rather than analyse them one at the time. Moreover, the Thermal, Hydraulic, Mechanical and Chemical (THMC) processes that may affect canister integrity are in many cases strongly coupled. One must therefore adopt an integrated approach covering both the components and the processes. However, the expected long lifetime of the canister itself may to some extent mitigate the potential adverse impact of many coupled processes on the radionuclide release performance because the strong initial gradients that drive coupled processes dissipate within the first thousand hundred years following repository closure (deMarsily, 1987). Two areas that are probably most crucial for canister integrity are:

- The corrosion behaviour of the canister influenced by the groundwater chemistry coupled with the extremely low hydraulic conductivity of the buffer.
- The mechanical integrity of the canister and buffer under THMC coupled processes in the bentonite-rock system.

This report is a summary of a workshop held in Sweden in November 2002, which addressed the above mentioned issues. The first part of this report is a synthesis of working group discussions at the workshop, and the other main part contains extended abstracts of presentations given by some of the participants. The focus of the workshop was the integrated treatment of the canister and bentonite buffer with respect to assuring long-term isolation of spent fuel. Other components of a KBS-3 type of repository, such as plugs, backfill, and rock reinforcement were not extensively addressed. The "isolation" that might be provided by a defective canister, resulting from the long-time frames needed to establish a continuous water pathway between the waste form and the near-field rock (e.g. Takase et al., 1999), was not considered.

The Swedish programme for a spent-fuel repository is now approaching the licensing phase, with a few years before submittal of license applications for construction of an encapsulation plant and subsequently for the construction of a repository for spent fuel. The Swedish Nuclear Fuel and Waste Management Company (SKB) has suggested a time frame, based on the time needed for the required development of the barrier-, system components, and the ongoing site investigations in the Forsmark and Oskarshamn municipalities. The Swedish nuclear power inspectorate (SKI) and the Swedish radiation protection authority (SSI) need to be prepared for the future reviews of these license applications, which all include a performance assessment (PA) related to long-term safety.

The planning of this workshop started soon after the completion of a similar workshop held in Sweden 2001, covering radionuclide transport modelling (SKI Report 02:30). The need of a similar effort focussing exclusively on the engineered barrier system and its isolation function became apparent at that time. The workshop reported here should be considered as a part of comprehensive strategy that SKI will use to prepare for future license applications from SKB. This strategy is discussed in SKI Report 02:30 (Sections 5.1 to 5.6).

## 2. Objectives

There are two main objectives of the workshop: 1) to identify important fabrication, installation and performance issues that could adversely impact the isolation function of the EBS, and 2) to generate a list of actions and needs that are practical, given the current regulatory review framework in Sweden. Such actions are likely to focus on specific EBS issues identified in the present workshop, and may for instance involve working groups examining more specific issues identified as being particularly important. The relatively large scope and preliminary nature of this workshop necessitates the focus on identification of issues for further consideration, as opposed to an attempt of resolving as many issues as possible. Although SKB provided presentations about ongoing work at the workshop, (in fact that most participants at the workshop already had a reasonably good overview of the SKB programme) details concerning the present SKB coverage of certain questions and issues raised at the workshop were to some extent unknown. The many suggestions and comments included in this report should therefore not primarily be interpreted as criticism of the present SKB programme, but rather as a reminder of the important aspects to consider in the preparations for future PAs, as well as their reviews. Viewpoints presented in this report are those of one or several workshop participants and do not necessarily coincide with those of SKI.

## 3. Format of the Workshop

The workshop contained presentations about ongoing research projects related to canister integrity (Appendix 3), presentations by SKB covering ongoing work and recent developments since the SR97 performance assessment, and finally, working group sessions. This report is mainly a synthesis of the notes that the three working groups provided after the workshop (SKI, 2002). The report also reflects the discussions in the plenary session summarising the results of the working group sessions and, to a limited extent, also some discussions after the workshop among some of the participants.

The three working groups were selected such that each of them could provide the broadest possible coverage in terms of competence in various areas (for a list of workshop participants, see Appendix 2). As a background for group discussions, the members had been asked to study the base scenario (the scenario that essentially illustrates SKB`s view of canister integrity) in SKB`s most recent performance assessment (SR97) prior to the workshops. The idea was not to once again review SR97 but rather to use it as a starting point for the discussions.

In the first of the two working group sessions, all the groups were given the same task, namely to go through some questions and a list of issues prepared with the SR97 as a basis (Appendix 1). In the second session, each group was given its own time scale for the evolution of a spent fuel repository and was asked to provide more a more detailed description of important issues for the time scale under consideration. The three time scales were:

- Fabrication and pre-closure period: initial state of the EBS system, emplacement, repository operation, possible defects or flaws in barriers arising from fabrication, handling/ transportation, and inspection of buffer and waste package (i.e., sealed canister with spent fuel inside) that compose the EBS, as well as consideration of perturbation to ambient conditions at the site arising from repository excavation and construction, (Sections 3 and 4).

- Initial thermal period: subsequent evolution in the physicochemical conditions of the EBS and surrounding near-field portion of the site, caused by coupled thermal-hydrological-mechanical-chemical (THMC) processes driven by strong gradients in temperature, head, stress, and concentration (Section 5).
- Long-term isolation: period of EBS isolation performance characterised by a decrease in gradients and restoration of near-ambient site conditions within the EBS and near field, as well as climate change (Section 6).

The first remark to make regarding the outcome of the workshop is that it was profitable to have more than one group addressing the similar, overlapping issues that span two or more of these time periods. Notes from the groups were complementary even for the first session, during which all the groups were asked the same questions. Points from the groups that overlap were noted, and the overlap highlights that these issues, with high degree of confidence, can be regarded as key ones. In the preparation of this synthesis, however, the overlap has been removed. Also, we have not noted which of the groups said what, but rather only noted that one of the groups identified a particular issue.

We have not made any significant efforts to quantitatively assess what will be important and what will not be at the performance assessment level (this to a large extent depends on the proponents' priorities). In the preparation of the synthesis, we rather focussed on identification of issues that appeared to be important at a more basic system understanding level. The goal was to obtain a reasonably complete summery of the issues that emerged from the workshop, with the detailed prioritisation of issues for further consideration postponed to later stages. The only items that were removed were issues for which notes from the workshop were so brief that the context could not be completely reformulated. On the other hand, the description of some of the included issues has been expanded afterwards, to give the reader a better understanding of their context.

Issues on the three time scales are presented in Sections 3-6 as indicated under the three bulleted points above. Section 7 comments on treatment of canister integrity in systems and scenario analysis. Section 8 includes a brief discussion about the possibility to use independent modelling as support for future regulatory reviews. This synthesis report ends with some conclusions and discussions in Section 9.

# 3. Initial State of Repository System: Characteristics and Quality of EBS Components

## *Canister: quality of copper shell and insert*

The sealing of the copper canisters will be a critical step for achieving the expected long-term safety of the KBS-3 concepts. At the time of licensing there must be data or information providing defensible basis for evaluation of the probability of initial through-going defects postulated as part of the SR97 performance assessment (in SR97, these were assumed to have a cross section of 1 mm$^2$). A very low probability of such defects is expected and has to be demonstrated. In addition, a few of the participants at the workshop expressed concern about the fact that long term implications of smaller defects were not discussed in SR97. These would not be through-going and give rise to immediate leakage, but they nevertheless need to be considered in the analysis of chemical and mechanical processes affecting long-term isolation. SKB should analyse and select acceptance criteria for small defects, as well as demonstrate the capability to detect and characterise such defects.

The welding method is expected to have a profound influence on the likely type and occurrence of defects. For electron-beam welding, concern was expressed about the variability of the weld seam quality and the prospects of understanding and controlling the reasons for this. For friction stir welding, the possible influences of wear debris and its orientation, as well as residual stresses, were mentioned as open issues. Regardless of the choice of the welding method, SKB should, in the context of material testing, use materials that correspond to the weld seam rather than only the bulk material, since this is likely to be the weakest part of the canister. However, this does not mean that specifications only need to address the weld/seal areas (e.g. specifications requiring fine grain for areas of welding). The quality requirements for central areas of the base and lid of a canister also need to be addressed.

The characteristics of the iron insert and its implications is equally important as the outer copper shell, since this is the component providing the required mechanical strength. Its properties may be influenced by variability in grain-size distribution from one end to the other. One workshop participant proposed that the material properties (specifically grain size) may not be uniform along the length of the insert. Rather, there might be some gradation in material properties from nodular iron to graphite flakes, with corresponding differences in mechanical performance. To establish the nature of such a gradation or any other material defect, workshop participants recommended that some form of non-destructive testing of the iron liner should be conducted prior to sealing. In addition, to support the non-destructive testing data, it may be worthwhile to cut up several liners, examine them for defects and test them for mechanical toughness**.** Further, to address possible defects in this insert, SKB should develop acceptance criteria for manufacturing defects, with a strategy for ensuring specified limits for stress response.

Finally, there was a discussion about tolerances in the diameters of the copper shell and the iron insert. A point was raised that the rather small difference (1 mm) between the shell and the insert may create problems during serial production. Nevertheless, the void space should be small to limit the creep deformation of the copper shell.

## *Bentonite buffer: quality and composition*

In the Swedish programme, the quality requirements for the bentonite buffer have not received as much attention as those for the copper canister, in spite of the fact that the bentonite buffer is an equally important component to ensure long-term safety. This is, to some extent, understandable, since the quality requirements on the buffer will probably not have to be as precise as for the canister. On the other hand, these requirements are more diverse. Examples of the buffer requirements utilised in PA are that it should:

- protect the canister against shear movement of the rock
- provide Eh (and pH?) buffering
- eliminate advective solute transport
- eliminate transport by colloids
- eliminate microbial activity near the canister surface
- facilitate transport of hydrogen gas that may be produced by corrosion of the iron insert.

Some of the workshop participants held the opinion that the requirements for the buffer need to be updated and reviewed, based each of different functions for the buffer that are assumed in the current PA. These requirements would include the acceptable compositional ranges for the desired components (e.g. smectite, pyrite), as well as the maximum contents of various impurities. Other factors that could influence the long-term buffer performance, such as the density and water content of manufactured bentonite blocks, also need to be closely monitored. A quality programme needs to cover all aspects of the buffer features and safety functions. In developing them, there should be greater opportunity to utilise information and results from other radioactive waste management programmes, since the bentonite buffer is an almost universal component of future spent-fuel repositories (except the Yucca Mountain Project, USA), as compared to the copper canister.

## *Other EBS components*

The required functions of the backfill were briefly discussed, for instance, its role in keeping the buffer and canister in place, and avoiding the formation of potential pathways for groundwater flow. Some concern was expressed about the fact that SKB seemed not to have arrived at a firm decision about what material to use, in spite of the substantial experimental efforts using a mixture of crushed rock and bentonite at the Äspö laboratory. Regardless of which material SKB finally selects, there is little time left before the submission of licensing applications to demonstrate the intended functions of the backfill with long-term full-scale experiments. The present strategy for addressing the backfill in PA may have to be reconsidered, or alternatively, the sensitivity of various assumptions about the backfill may need to be better demonstrated (e.g., concerning the assumption that the backfill will have virtually the same hydraulic properties as the surrounding rock for up to 1 million years). Long-term experiments should nevertheless be initiated as soon as possible, to build up the confidence needed for e.g. sealing deposition galleries, and eventually the entire repository.

It is noted that large amounts of concrete are likely to be used in repository construction, for instance, as grout and plugs. One of the working groups believed that these future repository components have received fairly little attention in the Swedish programme. The potential for this concrete to chemically alter the buffer and backfill should be analysed. In addition, if cement additives are to be used, their possible influences in the repository environment need to be fully understood. Questions exist concerning the properties of concrete at higher temperatures and concerning the ”lower-pH” cements that were mentioned by SKB during the workshop.

## *Handling of EBS components*

In addition to the manufacturing processes, the handling and storage of EBS components need to be considered. Storage on the surface or in the repository environments will initiate corrosion of copper canisters and may also affect the moisture content of bentonite blocks. Conditions and maximum time frames for storage should be specified. The impact of waste handling and transport could influence the mechanical properties of the the bentonite blocks.

The actual moment of deposition canisters and buffer, which was also considered as part of the handling, would involve small tolerances and potential for mistakes. The consequences of impact between canister and buffer need to be addressed. Consequences of handling of these components are closely related to human mistakes, discussed below.

## Human mistakes

Members of one of the working groups specifically emphasised the need for SKB to acknowledge that human mistakes do occur, and therefore incorporate this reality explicitly in to the systems and scenario analysis. When the more specific and detailed plans for manufacturing EBS components and repository operation have been developed, it may be possible to conclusively rule most of them out. However, at this preliminary stage, identification and analysis of possible human mistakes are, unless proven otherwise, important in the assessment of long-term safety, and may help to identify particularly sensitive steps of handling and operations. Human mistakes may, for instance involve:

- contamination of repository (see Extraneous materials below)
- exceeding fuel loading specifications (e.g., too high thermal output)
- error during canister/buffer emplacement (e.g., resulting in non-uniform buffer thickness)
- use of EBS components that fall short of specified quality standards (e.g., damaged bentonite blocks)
- large variability in EBS component quality
- non-destructive testing of EBS components not working as intended
- use of deposition holes with properties outside the specified range
- defective canister close to an exploratory borehole, without or with poor seal

## Extraneous materials

The main repository components should not be included in the category “extraneous materials”, although they are, strictly speaking, extraneous in the natural rock environment. Extraneous materials are intentionally or unintentionally deposited chemical or biological substances that may contaminate the repository environment and may exert a negative influence on various chemical and biological processes. These components could be released as a result of human mistakes and failure (e.g. lubricating oils from vehicles operated in the repository). Examples of the effects of extraneous materials are as complexing agents (cement additives or other organic compounds) or nitrogen compounds affecting copper corrosion (blasting gases, human wastes etc.). Microbial processes could possibly both increase and decrease the influence of various extraneous materials. Participants at the workshop regarded the consideration of extraneous materials and their impact as an important element of PA.

## 4. Early evolution of repository after sealing of repository galleries

Soon after canister deposition has been completed with a gallery, the deposition tunnel will have to be backfilled and sealed and deposition will continue in an adjacent gallery. This means that part of the repository will be operational while other parts are in a transient phase (e.g., sealed galleries). This transient phase could last up to more than 50 years before the repository as a whole is backfilled and sealed. Although the extent of adverse processes occurring during this limited time frame might be small, analyses of such processes materials and time scales should be considered in the performance assessment. Moreover, suitable terminology is needed to describe this evolving system, e.g., precisely what is meant by the pre-closure, initial and long-term conditions for the safety assessment?

A range of processes could affect the initial conditions for the assessment of the post-closure phase. The most important initial processes are probably the resaturation of the bentonite, which is coupled with evolution of the thermal field and the mechanical influences on the canister and near-field rock. The assessment of these processes is very similar to the post-closure phase and will be discussed also in Section 5.

### *Processes occurring during operational phase*

A process that would begin immediately after deposition of a canister and buffer in its deposition hole would be "chemical resaturation" (i.e. restoration of the original groundwater chemistry that has been perturbed by  repository construction and operation), with a return from oxidising to the original reducing conditions in the buffer, backfill and near-field bedrock. The reducing capability of the pyrite in these environments may be the key in this process, or possibly microbial activity in the intruding groundwater. Establishing the time frames for chemical resaturation is of significance when assessing the magnitude of initial copper canister corrosion in an oxidising environment (during transportation, storage and the initial disposal conditions). This would require, for instance, an assessment of the amount of oxygen in the system and the possible transport pathways for oxygen. One of the working groups recommended that SKB monitor oxygen consumption in the buffer during realistic full-scale experiments.

The period of oxidising condition in the buffer may well be much shorter than the time frame for hydraulic resaturation, but has to be considered as a component in the overall assessment of canister corrosion. Potential for stress corrosion cracking would exist if the oxidising condition occurred simultaneously to tensile stresses. Possible effects from the oxic film that would form on the surface of the canisters have to be considered.

Hydraulic resaturation would also begin soon after canister and buffer deposition, although it may likely be only partially completed by the time of repository sealing. The possible effect of an adjacent open tunnel on resaturation rate within a backfilled tunnel was discussed during the workshop. It was concluded that resaturation should not only be considered at the scale of a deposition hole, but also of the scale of the entire repository to reflect the fact that different parts will be open and closed at the same time. One workshop participant wondered whether restoration of fluid pressure around tunnels could affect the strength of the rock mass.

Finally, the upconing of saline groundwater during the period of repository operation was discussed. SKB has in particular focused on its influence of buffer swelling and suggested an upper limit of 100 g/l. This limit is very high, and it may be necessary for SKB to consider the effects of groundwater with considerably lower salinity. Possible implications that need to be looked at are the function of the backfill, corrosion of rock support, and any influence on equipment used for monitoring or repository operation. Recent results also suggest that the issue of copper corrosion under saline conditions needs to be revisited (see abstract by Bojinov et al in this report).

## *Long-term experiments and Monitoring*

Long-term experiments can be conducted before and during the operational phase of a repository. Currently, the prototype repository and long-term buffer test have been initiated at the Äspö hardrock laboratory. The objective of these experiments is to obtain the knowledge and confidence necessary for licensing the construction of the repository, the active operation of the repository, and the sealing of the repository. Many workshop participants believe that these experiments would establish a very significant basis for the future licensing decisions. However, concern was expressed about the problems with the heaters in the prototype repository, and that failure of the heaters would eventually occur. SKB was therefore recommended to seriously consider whether or not some type of back-up experiment is needed. Over the long time frames of the various licensing steps, the opportunities to initiate meaningful long-term tests will gradually diminish at later stages. It should here be noted that one of the working groups was more sceptical about the usefulness of long-term experiments. They believed that no hope exists for obtaining the required results, since time frames will always be too short. Their opinion was that future decisions have to rely on a sound understanding of fundamental features and processes.

Apart from long-term experiments, monitoring of the sealed galleries was discussed. The approach must be to firstly identify the specific needs of monitoring and then design it with a balance between intrusive monitoring and meaningful data. Monitoring for release of radionuclides is not expected to give meaningful results, other than to enhance public confidence, since the time frames involved for nuclides to even escape from a defective canister would be too long. The consensus was that monitoring should rather be related to **performance confirmation** (performance confirmation is in the USNRC regulation 10 CFR Part 63 defined as a program of tests, experiments, and analyses that is conducted to evaluate the adequacy of the information used to demonstrate compliance with the performance objectives) and **long-term safety**, with examples being monitoring the resaturation of buffer and backfill, as well as thermal evolution. SKB needs eventually to develop a monitoring plan and, possibly in conjunction with this, a mitigation plan. Eventually, a monitoring plan also needs to be set up for the post-closure phase.

One of the working groups suggested that SKB should set up a demonstration tunnel, similar to the experience at WIPP, USA. The objective here is to have a filled tunnel containing canisters in deposition holes, with buffer and backfill in place - all representative of actual repository conditions. The group compared this option with the heater test in the Äspö prototype repository but concluded that the spent fuel needed to be emplaced. Only after emplacement could the internal state of the inside of a fuel canister be representative of degradation processes under a radiation field and realistic moisture conditions. Needless to say, problems with heating are not expected to be addressed. Such a demonstration project would require removal of a few canisters from their deposition holes before sealing the repository. If judged meaningful, these canisters could effectively be sacrificed in the demonstration project by cutting open the copper lids and removing the insert and fuel assembly for detailed examination. Clearly, this working group felt that a demonstration tunnel would be a worthwhile exercise in performance confirmation, given the importance of the canister and its contents to long-term isolation. Additional discussion at the workshop focused on exactly what parameters relevant to long-term isolation would/could be monitored in this exercise. The conclusion was that over a few decades at least, data relevant to resaturation patterns within deposition holes, buffer swelling (including uneven swelling), interface characterisation, degradation, and corrosion processes, under high radiation and initial near-field heating conditions, could be gathered.

## 5. Evolution of Repository during Elevated Temperature Period, Up to a Few Thousand Years

One of the first remarks made during the introduction of the working group session was that it is insufficient to discuss individual processes and the evolution of single EBS components one by one. A few workshop participants felt that the provided issues list (Appendix 1) gives that impression. The recommendation was therefore to focus on **the coupling between processes**, e.g., thermal-hydrological (resaturation), chemical (corrosion) and mechanical processes. Thus, the emphasis should be on the **integrated system**. For example, the analysis of the long-term integrity (mechanical stability) of the copper canister by necessity needs to include consideration of the various processes affecting the buffer. All of the working groups emphasised the importance of continuing efforts to develop and improve **coupled THMC modelling**. One of the working groups pointed out the importance of the representation of interfaces (canister-bentonite, bentonite-rock) when modelling the integrated Canister-Bentonite-Rock system (C-B-R), and that there should be the capability to account for two-phase flow across these boundaries.

Another general comment was that **heterogeneity** and **variability** of the system should be regarded as being particularly important in the context of uncertainties. In other words, considering mean properties alone is insufficient. This heterogeneity and variability can be exemplified by the variability of the hydraulic properties of the deposition holes and the thermal outputs of the canisters.

In this section, we summarise the most important comments from the working group sessions with emphasis on thermal, hydraulic, mechanical, chemical and radiation effects, respectively. For each of the effects, couplings to the other effects are highlighted.

## *Temperature effects*

One of the working groups had a detailed discussion about how canister surface temperatures, $T_{surface}$, will develop and the uncertainties associated with such predictions. SKB has specified the maximum permissible $T_{surface}$ to be 90ºC, which will be achieved by adjusting the thermal loading of the canisters (by selection of fuel bundles) and the separation distance between the deposition holes. The groups emphasised the importance of explicitly addressing uncertainties in the prediction of $T_{surface}$ evolution and in particular the peak $T_{surface}$. They had the opinion that there might be significant variability in the early evolution of the surface temperature, owing to the variations in the **hydraulic** resaturation of different deposition holes. The difference in hydraulic properties in between deposition holes may therefore influence early thermal evolution, since thermal conductivity of bentonite is a function of its water content. The **coupled** nature of these processes is apparent, since the canister surface temperature, $T_{surface,}$ in turn has an effect on the resaturation process.

The group also discussed the thermal evolution on the repository scale and concluded that the **mechanical effects** on the near-field rock should be assessed. The permeability of the near-field could change due to thermal stress. In addition, the question was raised concerning if and when, the thermal fields for adjacent boreholes could impinge. Would this cause heterogeneity in the large-scale thermal field, which in turn may cause significant local stresses? For the repository scale thermal evolution, the mechanical influence of the cooling-down period should also be considered.

In the human mistakes category of events, a question was raised about the consequences of a ”mistake”- off normal fuel loading of a canister (e.g., more than one MOX assembly per canister).

The other two working groups did not discuss thermal effects in any detail, but rather concluded that the principles behind modelling thermal evolution are very well established and that there should be little uncertainties in determining thermal conductivity and heat capacity for the relevant materials.

## *Hydraulic effects*

All of the working groups devoted considerable attention to the question of buffer resaturation. This could possibly be the single most important question regarding the early evolution of the repository components. There are at least two aspect of this that need to be addressed in detail: one concerns the time scale to reach full saturation and its variability and the other concerns the mechanical influence on the canister caused by an uneven resaturation and swelling.

The problem with the duration of the resaturation period is that it may last much longer than what has been anticipated. If this indeed turns out to be the case, SKB needs to address the question: are there any significant impact on long-term safety whether the resaturation lasts a few years, a few decades, more than one hundred years or possibly even a thousand years? The resaturation process will affect the **thermal** properties of the buffer and may therefore influence the peak canister surface temperature (as discussed above). There may also be **chemical** influences on the buffer due to a higher temperature, which may in turn affect its **mechanical** properties.

Experimental data collected in some large-scale experiments (Febex Mock-up Test) suggest that bentonite hydration proceeds at a rate lower than expected on the basis of conventional flow analysis (see abstract by Alonso in this report). Some possible physical phenomena, such as the existence of a threshold gradient below which no flow takes place, modification of clay microstructure, and thermo-hydraulic couplings, may explain the observed retardation. An additional phenomenon that may be significant is the desaturation of the near-field rock, which may occur simultaneously with the resaturation of the bentonite and as a consequence of a low water supply from the bedrock. There is, in general, limited experimental information about the nature and significance of these phenomena. On the other hand, they have important consequences for the long-term saturation of the barrier. In particular, the threshold gradient effect may imply that barrier saturation is not fully achieved even in the long term (see abstract by Alonso in this report). Long-term saturation requires further investigation, which should be supported by detailed laboratory testing and the interpretation of medium- to long-term tests at a larger scale.

The hydraulic characteristics of individual deposition holes may result in vastly different scenarios in terms of the resaturation of the bentonite. Conditions in the deposition hole may vary from a steady flow of water to practically completely dry. A very wet borehole could imply a poor performance regarding radionuclide transport (Andersson et al, 2000), and a large-aperture fracture intersecting a deposition hole could result in significant bentonite extrusion and erosion. On the other hand, a very dry deposition hole could severely affect the resaturation of the bentonite and possibly lead to unforeseen changes in the bentonite. Understanding how of the deposition hole hydraulic connections with the fracture system in the near-field rock is of major importance. SKB may need to revisit the question of “respect distance” to water conducting features of different types, as well as exploratory boreholes.

A strategy for dealing with the two extreme cases described above (very dry and very wet holes) should be formulated and executed, proving that the integrity of the barriers will be secured. In addition, SKB has in a different context mentioned the possibility of an artificial wetting of the buffer from the tunnel above. If credit is to be taken for this option of resaturating the buffer, mathematical modelling and/or some type of demonstration experiment should be considered.

One of the working groups discussed the issue of non-uniform wetting of the buffer. Uneven wetting of the buffer would result in uneven swelling, with the resultant potential of highly uneven swelling pressure focussed on a few locations on the canister surface. This would cause **mechanical effects** such as localised stress transfer to the canister. This could result in movement, tilting or deformation of the canister. The group believed that uneven wetting/re-saturation was a realistic possibility in a fractured rock environment wherein the fracture patterns (influx of groundwater) will vary from one depositional hole to another. The bentonite swelling could also have a significant effect on the near-field rock, with the possibility of significant deformation induced on the rock fractures changing the permeability and the nearby flow field.

The issues of uneven wetting and resultant mechanical stresses, as well as uneven movement of the canister can be addressed experimentally. A mock-up of the canister-buffer-rock system (under thermal load) could be established; the buffer is subsequently resaturated on one side only, in this way, maximum canister movement could be determined. The possibility of canister movement causing a canister to rest on its edge could also be evaluated.

Working group discussions of the backfill evolution focussed on the potential for preferential flow through and neighbouring this material. The likelihood of backfill settlement and the formation of a preferential flowpath at the top of the backfill were regarded as a significant possibility. The underlying causes that were mentioned were an increase in groundwater salinity and poor compaction of the backfill. High salinity may also accelerate degradation of rockbolts, which might lead to some collapse at the top of drifts. The actual saturation phase of the backfill also needs to be studied.

At a repository scale, large volumes of saturated rock undergo a significant increase in temperature. This implies a water pressure increase caused by the different thermal expansion coefficients of water and rock, and a change in water density. Both effects lead to thermally induced water flow whose intensity and potential effect on the repository (and its dependence of some rock properties, such as porosity, structure, and permeability) should be evaluated by appropriate modelling.

One of the groups mentioned the hydraulic influence of the excavated damaged zone (EDZ). The EDZ is created during tunnel excavation. SKB has estimated that at most 0,5 m of the rock mass close to tunnel drifts may be affected. However, the group regarded this to be a minor problem.

## *Mechanical effects*

A potential consequence of SKB´s canister design, with the mechanical strength provided by the insert is that the copper shell will be subjected to creep deformation. The elevated temperatures would, to some degree reinforce this creep deformation. The two causes of creep of the copper shell that were discussed during the workshop are (1) a possible uneven swelling pressure focussed on a few locations on the canister surface (se above) and (2) deformation of the small gap between the shell and the insert. The former may be most significant, since compressive creep was regarded as less damaging compared to tensile creep. The group’s concern therefore focussed on shear deformation under bentonite swelling pressure, and subsequent flexing of the canister shell. The time scale for the analysis of creep behaviour has to be coupled with the analysis of the **hydraulic** buffer resaturation. There is also potential coupling to **chemical effects** with corrosion problems caused by shear deformation.

One group in particular emphasised that the creep properties of copper are not well enough known and further work will be needed in this area. It was noted that realistic **creep data** for the copper canister are not available. Creep data for loads more than100 MPa exist, but extrapolation to loadings less than 100 MPa is not acceptable, particularly for phosphorus-loaded copper. What is required, therefore, are creep data for loadings less than 100 MPa to identify an accurate mechanical response, i.e. a stress relief profile.

The mechanical effects on the near-field rock properties were rather briefly discussed, although there may be significant effects on the **hydraulic properties**. A relevant example might be that the bentonite swelling pressure opens up fractures intersecting a deposition and alters the flow field. Other reasons for a mechanical influence on the rock mass may be **chemical** degradation of rock support, thermal expansion, and differential land uplift. Mechanical effects related to tectonic events are discussed in Section 6.

One group wondered whether or not the mechanical effect on fractures in the buffer had been sufficiently studied and whether any evidence existed that proved that such a fracture would self-heal during bentonite swelling.

In the context of canister sinking in the buffer, and/or uneven movement of the canister, concerns that some participants raised were extrapolation using empirical relationships, the possible time-scale of relevant experiments and consideration of realistic near-field conditions. The density range of compacted bentonite is an important factor for acceptable performance of the base of the buffer (increasing the density of the buffer at the base of the canister will help counteract the load). Case studies (modelling) were recommended.

In order to address the extent of bentonite extrusion into fractures and cracks in the near-field rock, one of the working groups recommended a characterisation of the saturation state of rock with regard to wetting of the buffer and its subsequent swelling and extrusion. The strategy of emplacement (horizontal vs. vertical) will affect this issue. Thus, swelling of the buffer under temperature and moisture gradients might be analysed for both the vertical and the horizontal direction, to cover a possible change in the disposal concept.

## *Chemical effects*

The main chemical effects related to the EBS concern the long-term transformation of the bentonite buffer and copper. These changes occur because these materials are not fully thermodynamically stable and would be transformed to, for instance, non-swelling clay minerals as well as copper sulphides. However, any significant effect resulting from these processes would be more severe in the time scale up to a million years, since they are expected to be very slow (see Section 6).

In the shorter time scale addressed here, it may be more relevant to consider chemical effects that do not require a large exchange of mass between the deposition holes and the surrounding groundwater. Two feasible mechanisms for copper corrosion are pitting corrosion and stress corrosion cracking. Presently available data suggest that these processes are most likely to occur only during initial oxidising conditions. However, one of the working groups recommended that more work was required to establish a firmer theoretical basis for explaining and understanding these processes before they can be ruled out for the subsequent reducing phase. In particular, one has to consider any insufficiently characterised water chemistry or biochemical parameters (e.g., acetogenic bacteria, acetate, organics) that are significant for pitting corrosion and stress corrosion cracking. A combination of different chemical parameters needs to be considered, as well as for stress corrosion cracking, the effective stress levels. The influence of salt precipitated or accumulated on the canister surfaces during bentonite resaturation phase was also briefly mentioned as a process that might affect canister corrosion.

The chemical alterations of bentonite considered most important during the thermal phase are the heating and possible cementation of bentonite particles close to the canister surface. This effect would be particularly important for the canister position with the highest thermal output and the case of an extremely long resaturation phase. A drying and hardening of the bentonite would affect its **mechanical** properties. A more general comment from one of the working groups was that the consideration of ion-exchange, pH-buffering (by calcite) and redox-buffering (by pyrite-ferri(oxy)hydroxides and ferrous/ferric ions in the octahedral sites of smectite) is not sufficient to satisfactorily explain the long-term bentonite alterations. It is essential that the more complicated alteration of bulk-sheet silicate phases is also predicted. A contributing factor for such alteration might be the reaction with hyperalkaline pore water from concrete within the repository.

Microbially catalysed processes may have an important effect on redox processes in the repository environment. Although microbial activity may be excluded from the buffer environment (due to very limited water activity), any microbial activity near deposition holes or backfilled tunnels would be significant, with an example being the microbially catalysed sulphate reduction producing sulphide ions by oxidation of extraneous organic matter or methane. Note that organic material would be introduced if crushed rock used for backfilling were stored on the surface for a significant length of time.

### *Radiation effects*

A few questions related to radiation effects were raised during the workshop. The most significant question concerns the influence of gamma radiolysis at the canister-buffer interface and its influence on Eh and copper corrosion. SKB had earlier stated that the impact of radiolysis and corrosion is negligible, but members of one working group wondered whether experimental data for both dry and wet buffer conditions existed that support SKB's claims. The possible influence of Compton radiolysis was also mentioned.

A final point up was about the internal canister corrosion and the potential role of nitric acid generated by radiolysis, in enhancing corrosion. The concern was that the sealing method may affect how much air and residual water is left in the canister.

## 6. Evolution of Repository after Thermal phase, Up to 1 Million Years

After the period of elevated temperature, one of the complicating factors disappears, namely a significant heat output from the fuel. However, several other long-term factors should be added with the most important one probably being the influence of the different climate stages, changing from present day conditions to permafrost, to glaciation, and back to temperate conditions through the next glaciation cycle (covering approximately 100 000 years). The transition to a colder climate could have temperature, hydrologic, mechanical and possible chemical (THMC) influences on the repository conditions. Some of these were discussed at the workshop and are summarised below.

In the even longer time scale of up to 1 000 000 years, the repository will be subjected to a series of glaciation cycles. These time scales are hard to comprehend, and one ought to be cautious in any claim that processes can be predicted for such long time scales. However, as long as there is a sound understanding of basic physical and chemical processes as well as knowledge from previous glaciation cycles, participants believed that reasonable conclusions about limiting cases could still be drawn. For all processes related to the long-term changing climate conditions, it need to be analysed whether any influence on the repository would be accumulative over the long series of glaciation cycles, or whether the system would reach an equilibrium state for each climate period and then alternate in between them.

## *Temperature effects*

One of the working groups focussed on the issue of permafrost. It was noted that permafrost down to the repository level was excluded in the SR97 safety assessment, but not in the SKB R,D&D program from 2001. The group recommended that two cases should be looked at: one considering permafrost down to repository level, and the other case considering the permafrost not reaching repository level, but forming a lid on groundwater flow and chemistry. The former case was regarded as most likely to occur at a rather late stage, at least 50 000 years from present day. Assuming that this case cannot be ruled out conclusively, the group recommended that the possible freezing and thawing of bentonite should be investigated in more detail. To gain confidence regarding this matter, it would be beneficial to perform laboratory experiments on compacted bentonite and "backfill", under saturated conditions and under pressure, through a freezing and thawing cycle.

## *Hydraulic effects*

The change to colder climate, permafrost and future glaciations will have a very profound influence on hydraulic conditions both within the repository and on a larger site scale, including the extreme example noted above of permafrost down to repository level. Even the changing flow rates and recharge/discharge patterns (flow directions) associated with climate change would influence the mass transfer mechanisms near deposition holes and probably the groundwater **chemistry**. These large-scale changes have an important influence on EBS evolution, but were regarded as essentially beyond the scope of the workshop.

## *Mechanical effects*

An issue that was, not surprisingly, debated during the working group session is the likelihood that a large disruption of the near-field rock may affect canister integrity. This has previously been one of the most frequently discussed issues related to long-term safety of a KBS-3 type repository in hard rocks. In particular, one of the working groups discussed the increased potential for earthquakes during the deglaciation phase, which has been suggested. SKB was recommended to examine in detail, the influence of the buffer canister under a shear movement of 0.1 m along a horizontal fracture intersecting a deposition hole. For this, SKB should use mathematical modelling (a calculation case discussed by SKB during the morning session). The worst case to consider would be if the bentonite were dry or hardened through **chemical** or **thermal** alteration (rock-like behaviour).

One of the groups also suggested that the experimental information should be gathered using destructive testing. SKB was encouraged to investigate the possibility of conducting some type of test with a model canister and buffer to simulate earthquake events. A collaboration and/or information exchange with the Japanese program was recommended, since JNC has specifically worked on this issue.

### *Chemical effects*

The chemical effects on the EBS system that can be regarded as most detrimental are illitisation of the smectite phase in the bentonite buffer through potassium from the groundwater and general corrosion of the copper canister by sulphide ions from the groundwater. However, the extent of these two processes can probably be constrained by mass-balance arguments even in extremely long time scales dealt with here. Nevertheless, the corrosion of copper in highly saline conditions needs to be studied further (see abstract by Bojinov et al.). Buffer loss through formation of bentonite colloids could also possibly be a significant effect for conditions of unfavourable groundwater chemistry, high flow rates, and the extremely long time frames.

The two long-term processes related to groundwater chemistry evolution discussed during the workshop were the change in groundwater salinity as a result of climate change and the possible intrusion of oxygenated groundwater during deglaciation. These are related to **hydrological** processes, but could have a pronounced influence on chemical conditions at repository depth. Also, permafrost could influence salinity through freeze-induced salt exclusion. The detailed analysis of geochemical stability and potential for groundwater chemistry alteration was regarded as beyond the scope of the workshop.

One of the working groups recommended further experimental work related to barrier integrity using very saline groundwater (canister corrosion, effect on buffer and backfill). There seems to be a very limited amount of data available on these rather extreme groundwater compositions. The SKB in-situ tests do not involve saline groundwaters, which are not available at the Äspö HRL.

# 7. Treatment of Canister Integrity in Systems and Scenario analysis

In the formulation of scenarios for performance assessment, decisions must be made regarding the treatment of the whole range of processes that may directly or indirectly influence canister integrity. The importance of the various issues discussed within this synthesis cannot be fully judged before these decisions have been made. It is therefore possible that some aspects of the EBS that may appear as problematic from a system analysis level can be obviated in the full context of performance assessment. Although evaluations of different issues in the performance assessment context were neither systematic nor detailed, some limited aspects of this were discussed during the working group sessions. The following section briefly describes some aspects of EBS isolation in performance assessment, starting with a summary of approaches that has been previously utilised.

In the SR97 performance assessment by SKB, failure of the copper canister was only assumed to occur as a result of initial through-going defects with a small probability. In the much earlier performance assessment KBS-3, SKB included a general analysis and discussion focussing on pitting corrosion as the key mechanism for canister integrity. Based on a conservative interpretation of this analysis, they assumed that the canisters would be penetrated according to a distribution covering the time span of 100 000 to 1 000 000 years. Performance assessments for most other spent fuel programmes typically involve a much shorter period of a few thousand years, during which canister integrity is assumed. These time scales for canister (or waste package) isolation and subsequent penetration are typically justified by corrosion rates and the thickness of a steel or an alloyed canister.

The key decision in the analysis of scenario-initiating FEPs (Features, Events and Processes) affecting canister integrity is the judgement whether they can be regarded as: (a) likely to occur, (b) improbable but possible, or (c) if they can be entirely screened out. The FEPs that could be regarded as likely to occur should be included as the basis for a main scenario, which is required by the SKI regulations for long-term safety (SKI FS 2002:1). Improbable-but-possible FEPs should be considered in the construction of a set of less-likely scenarios. In the overall compliance evaluation and necessary integration of scenarios, the justification of the probabilities for the less-likely scenarios is an element requiring careful attention. For screened out FEPs, the performance assessment must contain a comprehensive and defendable justification of why they do not have to be considered. A regulatory review has to pay particular attention to this part of the performance assessment. Finally, the consideration of relevant time scales should naturally be a key element in this process. For instance, general corrosion of copper is a FEP that will most likely result in failure of the copper canisters eventually. However, if this process with a high degree of confidence can be shown to be significant only in time scales much longer than those reasonable to consider (e.g. 10 000 000 years), general corrosion would not have to be a key FEP in a main scenario.

Table 1 shows a compilation of the processes that one of the working groups regarded as the prime candidates for directly influencing canister integrity. It has to be pointed out that also other processes previously discussed in this report may influence canister integrity, but for those processes omitted from the table, most probably only in an indirect way (e.g., by affecting the conditions under which the processes in the table could proceed). Providing a detailed discussion and analysis of the probability and significance of the processes in the table would not be possible, based on the rather broad and general discussions at the workshop. However, this will be a critical part of future performance assessments. It should be noted that we did not include any consideration of future human intrusion or human actions in the discussions about canister integrity.

**Table 1** Mechanisms (processes) that may directly influence canister integrity

| MECHANICAL INTEGRITY | CHEMICAL INTEGRITY |
|---|---|
| Pressure load | Chemical conditions |
| Residual stresses | Boundary conditions (for corroding species |
| Mechanisms: | |
| 1) Creep failure due to uneven bentonite swelling pressure | 1) Stress corrosion cracking |
| 2) Crushing due to hydrostatic pressure | 2) Localised corrosion |
| 3) Shear movement of host rock | 3) General corrosion |

Figure 1 shows a flow chart that may be useful as a tool for the selection of scenarios illustrating canister integrity. Based on identification of FEPs and possible initial states of the system, it needs to be decided whether or not any FEPs need to be considered as an initiator for a scenario that includes canister failure. The purpose of the next step in the flow chart is a reminder that even if no single FEP could by itself affect canister integrity, unfavourable combinations of FEPs should also be considered during the identification of scenarios. It should be emphasised that the consideration of each FEP one by one may not be a credible analysis of canister integrity. For instance, the likelihood of canister failure as a result of shear movement of the host rock would be a more likely reason for failure if the buffer had not been properly installed or had been subjected to any unfavourable alteration. Furthermore, alteration of the bentonite buffer would, in turn, be more probable if an unsuitable deposition hole had been selected.

The next step in the flowchart illustrates the decision whether or not fabrication defects of the canister have to be considered as a scenario-initiating feature, as was done in SR 97. This consideration is part of describing the possible initial states of the system, but is unique in that it directly defines a scenario with loss of canister integrity. The two last boxes in the flowchart contain two scenarios that may have to be considered regardless of the judgement that FEPs might affect canister integrity. The what-if scenario with radionuclide release aims at demonstrating that long-term safety is not entirely dependent on isolation as the single safety function. The importance of this aspect is mentioned in the SKI regulations for long-term safety. The final “scenario” covers the case for canisters that retain their isolation function throughout the whole period of PA consideration. Its main purpose is to demonstrate a reasonably realistic treatment of how various processes influence the EBS, without destroying its isolation function. This would be the justification for ruling them out as reasons for canister failure. One of the working groups believed that the term base scenario (terminology of SR97) is unsuitable, since it may imply that this by definition is the most likely scenario. The terms “as designed scenario” or “idealised scenario” were suggested as possible alternatives.

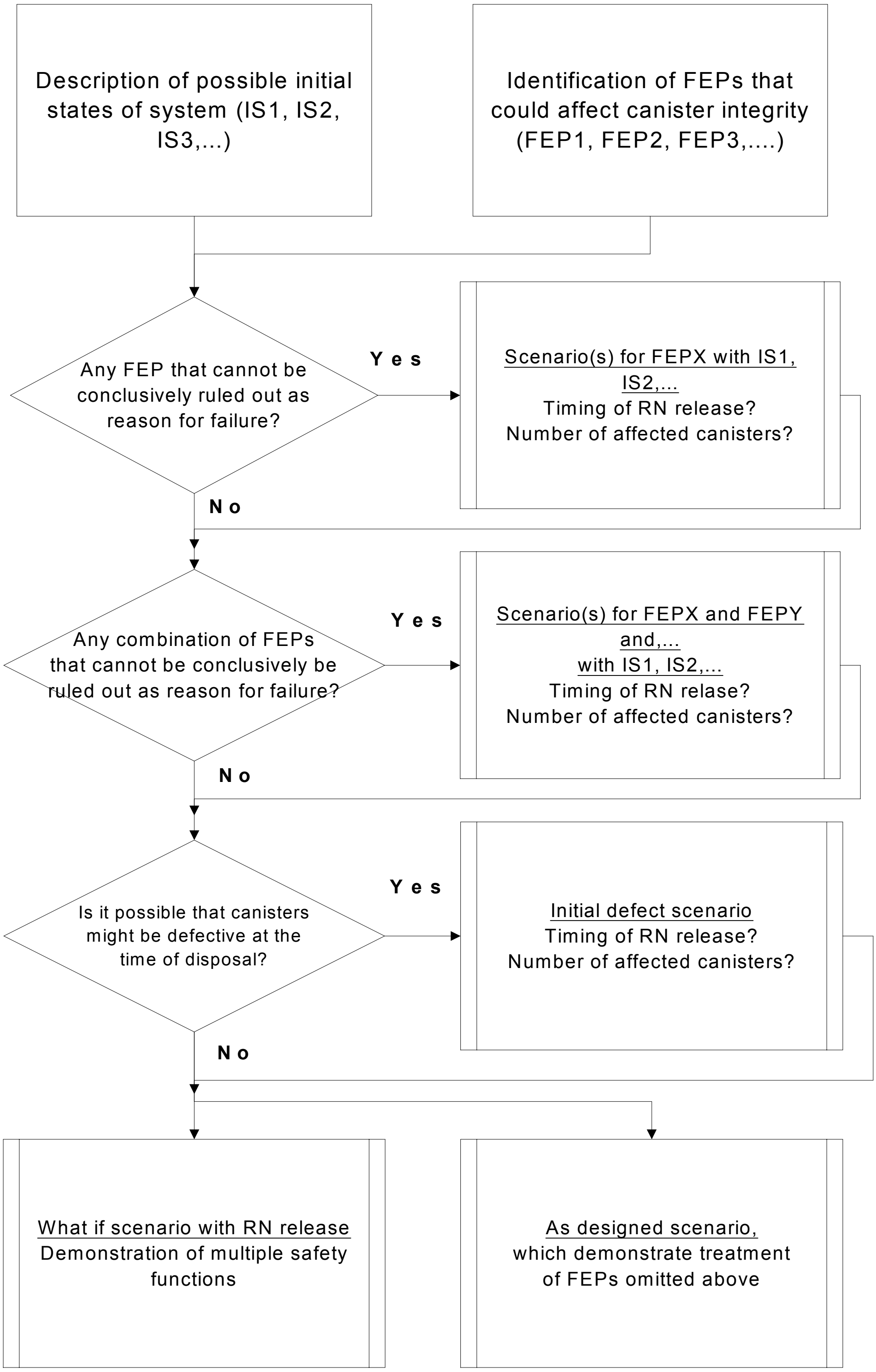

**Figure 1.** Flowchart for selection of scenarios

The probable nature of the initial state of the system received considerable attention during the workshop, especially the realistic state for the several thousand copper canisters. The workshop participants believed that a more realistic assessment is needed than the one presented in SR97. One should distinguish between the ideal initial state of the system, which could be described as the optimum state of the system based on the selected design with no unintentional deviations, from a realistic state of the system. A repository system operated over several decades will realistically deviate from its optimal state. Deviations may result from human errors, quality variations of engineering components and possibly an unpredictable heterogeneity of the system. It needs to be demonstrated that the nature and ranges of these deviations are reasonable, and that the safety implications are relatively small. The probability of a realistic state of system should by definition be high. One may also have to explicitly consider alternative unfavourable states of the system. This could include the state of the system after different types of human mistakes. To be included in this category, these mistakes should have safety relevance and result in a pronounced deviation from the ideal initial state. This category could be used to study the sensitivity of various phases of repository operations. Very low probabilities for such deviations need to be demonstrated.

A final point is that the timing of the expected radionuclide releases and the probable numbers of canisters affected are key considerations for any scenario involving canister failure. Experience from previous performance assessments shows that the failure of a single canister is not expected to result in unacceptable risk and dose (e.g. SKI 1997), but simultaneous failure of a multitude of canisters might. Doses would decrease, however, if canister failures were sufficiently separated in time without overlapping peak releases. In such cases, it is important that the spread in canister failure can be related to variability rather than just uncertainty (OECD NEA 2002). The burden of proof for demonstrating that all canisters would be intact for the entire period needs to be compared with that for demonstrating that most canisters will remain intact, and that a few canister failures would not result in unacceptable dose consequences.

## 8. Use of independent modelling in support of future regulatory reviews

Regulatory reviews need to be supported by independent modelling, in order to evaluate key technical issues and provide detailed comparisons with corresponding parts of the proponents performance assessment. This is an essential element to achieve sufficient scientific and technical depths of reviews, as well as ensuring the competence of the regulator. Since the resources of the regulatory side are always more limited as compared the implementor SKB, independent modelling can generally not cover all technical areas but must be limited to those that may controversial from some perspective or highly sensitive for repository performance. Thus, future reviews will most likely be based predominantly on expert judgement and less ambitious scoping calculations, complemented by independent modelling in key areas. In a previous SKI workshop, four different ambition levels of the required effort to deal with different issues were identified (SKI Report 02:30, Section 5.3):

- **Level 1**: requiring independent modelling (detailed expert review supported by application of independent modelling capability).
- **Level 2**: requiring scoping calculations (detailed expert review supported by limited scoping calculations to check SKB results).
- **Level 3**: requiring expert judgement (detailed expert review).
- **Level 4**: non-controversial.

The workshop participants were asked to identify areas that the regulator needs to deal with in a more comprehensive manner for future regulatory reviews (Appendix 1). According to the responses, a prioritised task for analysis of the isolation function should be THMC-modelling to address the evolution of canister, buffer, backfill and near-field rock. Workshop participants therefore recommended that current efforts in this area should continue, particularly with the purpose of improving integration of chemistry with previous THM-modelling.

A relevant example of SKI's engagement in THMC-modelling is the support for development of the ROCMAS and TOUGH-FLAC numerical codes within the DECOVALEX project (see abstracts in this report by Stephansson and Rutqvist). In the future, it is essential that the potential resource that these tools represent will be utilised in preparing for the review of coming license applications. However, the implementation of these codes would for resource reasons require careful evaluation. The finally chosen calculation cases should focus on only a few perspectives of the EBS evolution (which represent key issues), and possibly interpretation of SKB's long-term experiments. Example cases that were discussed include:

- bentonite resaturation under different hydraulic conditions
- uneven wetting of the bentonite buffer,
- two-phase flow across interfaces within the EBS system,
- long-term creep of copper under low strain conditions.

A screening and further evaluation of these would be required, as well as analyses of required code capabilities.

Another type of independent modelling is achieved when simplifications are used to a larger extent for a less rigorous sensitivity analysis of processes and parameters. This can provide a highly effective means for regulatory analysis provided that the solutions cover safety relevant features of the system and that rough comparisons can be made with more comprehensive modelling efforts. The work by Claesson (see abstract in this report), covering coupled heat and moisture flow in the bentonite buffer, is an example of this approach that may be extended and utilised in future PA reviews.

Participants expressed concern that coupled processes involving C (Chemical) has not been covered as extensively as those involving TH, TM and THM (Thermo, Hydro, Mechanical), in coupled modelling. It seems clear from these discussions there is a need for a more extensive integration of chemistry. There is comprehensive range of safety relevant issues involving the long-term chemical stability and degradation rates of the EBS components. The most safety critical issues probably involve canister corrosion and buffer alteration (i.e. smectite), coupled with THM processes, but there is a range of chemical processes also for other EBS and near-field rock components. At present, these phenomena are mostly treated in de-coupled manner or with a highly simplified coupling. However, non-linear effects caused by couplings of chemical and physical processes may be necessary to consider. The preliminary evaluation of the effects of the influence of the temperature dependent solubility of calcite and quartz in bentonite by Arthur and Zho (coupled THC-modelling, see abstract in this report) is an example that certain problems of this character can be analysed with available computer programmes. However, a broader and more comprehensive integration of chemistry in coupled modelling would require extensive resources. This could therefore be a suitable subject for an international collaboration between a range of organisations, in which SKI could participate.

Workshop participants recommended that scoping calculations should be used in support of regulatory review. This could involve using “back of the envelope” calculations or use or readily available computer programmes requiring little or no code development / modification. Participants suggested some subject areas and issues that could be covered with this type of simplified analysis. However, in order to utilise these suggestions effectively, more work is needed to define how these calculations could be formulated. In addition, scoping calculations would not always have to organised to the same level of detail as when SKI need to engage in the independent modelling work (described above). Scoping calculations could also be conducted spontaneously when a reviewer sees a particular need for it. A role of SKI would be to make sure that external reviewers get sufficient funding for not only reading and directly responding to SKB work, but also to conduct their own limited analyses.

Workshop participants also identified experimental or field analogue data as an urgent need to guide, constrain and enable credible analyses of THMC processes, as compared to further development of computer modelling. SKB and other repository programmes throughout the world are in the process of planning, collecting and reporting such data. SKI could to some extent compile and extract data from these sources, but there are no funding available to directly conduct this kind of data collection. SKI can, nevertheless, help point out those needs during the regular reviews of SKB’s R,D&D programmes, which are published every third year.

## 9. Conclusion and Discussion

The workshop was an important step in the establishment of a strategy to review the part of SKB’s safety case that is devoted to the demonstration of the isolation function of a future spent fuel repository. It must be restated that the emphasis was on identification rather than resolution of issues in this workshop synthesis. Subsequent steps therefore have to be taken within the Swedish regulatory bodies to follow up on this report and suggest activities within the regulators research programmes, as well as organise more detailed issue evaluation for different experts group. Ongoing and planned activities within the SKB programme that are related to the issues identified in this report would have to be reviewed in detail. The great emphasis of isolation of spent nuclear fuel rather than, e.g., radionuclide retardation and dilution, featured in the SR97 performance assessment, suggests that the Swedish regulators have to be prepared to review this part of the coming PAs in greater detail.

The specific features of the workshop that contributed to the rather comprehensive description of issues relevant for future licensing activities are:

- The combined consideration of the areas of the copper canister and bentonite buffer,
- the assessment of both chemical and mechanical aspects of EBS and canister integrity,
- the use of a published comprehensive performance assessment (SR-97) as a basis for discussions,
- the active participation by SKB providing additional information on recent developments.

There is an educational value for external consultants and researchers, as well as SKI staff, in addressing the broad subject areas relevant for the EBS isolation function. However, a broad coverage to some extent necessitates rather superficial view of the various issues under consideration. It should be noted that the descriptions in this synthesis can by no means be regarded as fully comprehensive, and that additional key issues may be identified in the SKB programme as well as future regulatory activities.

In coming years, a greater emphasis on EBS integrity issues can be expected within SKI's long-term programme for gradual development of review capability. In the autumn of 2004, an additional EBS workshop is planned, which will focus on EBS component quality and the expected initial state of the EBS. Subsequently, specialised workshops are planned for more detailed insight in selected areas, targeting issue resolution as well as identification.

A few of the technical issues that received considerable attention during the workshop are noted below:

- The performance assessment need to contain a description of the initial state of the system that can be regarded as realistic rather than idealised. In particular, the characterisation and statistical analysis of both large and small defects in the weldments of the copper canister has to be rigorous.

- The long-term experiments aimed at demonstrating feasibility of the KBS-3 concept have to be reviewed in more detail. It was suggested that SKB consider whether the present programme needs to be extended. SKB needs to present a plan for monitoring during repository operation. One of the working groups recommended that SKB should set up a demonstration tunnel in the repository, which would be dismantled and examined, with the purpose of performance confirmation prior to sealing the repository.

- The understanding of the resaturation phase for the buffer needs to be improved. Preliminary results indicate that the resaturation phase may be more extended that previously anticipated. In addition, an uneven resaturation of the buffer may result in localised stress transfer to the canister. All conceivable implications of an extended or uneven resaturation phase has to be evaluated, if they cannot be very convincingly ruled out, e.g. thermal gradients across the buffer may lead to mass transfer of chemical components, and consequently variations in thermal, hydrological and mechanical properties.

- More data is needed for evaluation of the buffer under unconventional conditions, namely with saline groundwater (because of saline water upconing, sea water intrusion or heterogeneous flows), and also under freezing and thawing conditions (extreme permafrost scenario).

- More work was recommended towards understanding the creep phenomenon and creep properties of copper. The occurrence of creep is a fundamental aspect of the integrity analysis. It is important as a direct consequence of SKB´s KBS-3 design, based on the mechanical support provided by the insert, which is surrounded by the softer corrosion barrier.

- On the issue of corrosion, general corrosion in highly saline environments needs to be addressed in more detail. If pitting corrosion and stress corrosion cracking is to be totally excluded, a strong and convincing case for ruling them out has to be included on the PA level.

- For very long time scales (up to and beyond 100 000 years), the implications of permafrost, shear movement due to earthquakes, and changing groundwater conditions (e.g. salinity) are particularly important issues to address on the PA level.

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## APPENDIX 1

## Topics included in SR97 Base scenario

1. Biosphere evolution
2. Decay of radionuclides (reduction of radiotoxicity with time)
3. Thermal evolution, canister scale
4. Thermal evolution, repository scale
5. Evolution of site-scale groundwater hydrology
6. Resaturation of buffer
7. Mechanical analysis of canister
8. Mechanical evolution of geosphere
9. Evolution of site-scale groundwater chemistry
10. Evolution of chemical processes in bentonite buffer
11. Corrosion of copper canister

## SKI EBS Workshop Topics

### *Not included*

1. Biosphere evolution
2. Decay of radionuclides (reduction of radiotoxicity with time)
3. Radionuclide transport (by the definition of the base scenario)
4. Analysis of spent fuel degradation

### *Included to limit extent mainly as boundary condition*

1. Evolution of site-scale groundwater hydrology
2. Evolution of site-scale groundwater chemistry

### *Added*

Selected parts of the Climate and Tectonics – earthquake scenarios

### *Subjects and issues retained from SR97 or otherwise judged to be relevant in spent fuel isolation context (subjects from center and outwards)*

1. Thermal evolution, canister scale
   - Initial heat output per canister
   - Thermal conductivity of engineering materials
   - Heat transfer at interfaces
   - Canister surface temperature (incl. criteria for selecting upper limit)
   - Impact of temperature on canister and engineering materials (thermal expansion, thermal cracking (if any), degassing (if any), etc.
2. Corrosion of copper canister
   - Corrosion during resaturation ($O_2$; hot and humid condition; localised corrosion max. 2mm)
   - Nitric acid corrosion (due to $\gamma$-radiolysis)
   - Stress corrosion
   - General corrosion (sulphide; limited by diffusion or GW flow)
   - Localised corrosion (sulphide; pitting factor of maximum 2 in SR97)
   - Effect of salt accumulation during resaturation
   - Effect of extremely saline conditions

3. Mechanical analysis of bentonite buffer and canister

   - Swelling under temperature and moisture gradients in the radial direction
   - Even swelling at the rock buffer interface and canister buffer interface (hydrostatic pressure and swelling pressure)
   - Uneven swelling at the interfaces (unsaturated and saturated conditions)
   - A movement of 0.1m along horizontal fracture (current SKB criteria for movement that may cause canister failure)
   - Bentonite swelling into fractures and cracks
   - Canister sinking in the bentonite buffer

4. Resaturation of bentonite buffer and backfill

   - Prediction of time to reach full saturation
   - Inflow of GW in deposition holes under temperature gradients (drying and wetting)
   - Movement of the interface between buffer and backfill
   - Water/moisture flows across the canister/buffer interface driven by the temperature gradients
   - Movement of canister during resaturation
   - Resaturation through backfill (credit taken in SR97 but not analysed)
   - Chemical bentonite alterations during cases of very slow resaturation

5. Evolution of chemical processes in bentonite buffer and backfill

   - Ion-exchange
   - pH and Eh buffering (calcite and pyrite weathering)
   - Alteration of montmorilonite (illitisation)
   - Cementation (during thermal phase)
   - Extrusion and erosion of bentonite (formation of colloids)
   - Swelling pressures at extremely saline conditions
   - Analysis of backfill (missing in SR97)
   - Effect of total pressure on chemical processes

6. Thermal evolution, repository scale

   - Thermal conductivity of rocktypes
   - Ambient temperatures and gradients
   - Effects of repository design (tunnels, ventilation during retrievability period affecting the source term on temperature distribution)

7. Mechanical evolution of geosphere (with emphasis on NF rock)

   - Mechanical interaction between rock mass and tunnels, buffer and backfill
   - Excavation effects and extent of EDZ
   - Thermal stresses with potential changes in NF permeability and porosity
   - Differential land uplift
   - Creep-induced deformation of deposition hole
   - Mechanical effects of glacial conditions on NF rock and canister hole
   - Mechanical effects of earthquakes on NF rock and canister hole
   - Development of super-lithostatic pressure in buffer pore water from earthquakes (due to contrasting rheologies of rigid rock and plastic buffer)
   - Temporal and spatial changes of unsaturated conditions in NF rock (dehydration due to ventilation, thermally driven steam formation etc.)
   - Flow and transport in the NF rock, such as EDZ and tunnel width

# APPENDIX 2

## Participants list

| | |
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| Eduardo Alonso | Universitat Politècnica de Catalunya |
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# APPENDIX 3

## Abstracts

# Abstracts

(In alphabetical order of first author).

- **ENRESA-FEBEX and Mock-up Tests – Lessons Learned and Outstanding Issues**
  Eduardo Alonso
- **Development of Coupled THMC Models of Buffer Evolution**
  Randy Arthur and Wei Zho
- **Creep and Creep Damage in Copper under Uniaxial/Multiaxial Loading**
  Pertti Auerkari, Stefan Holmström and Jorma Salonen
- **The Effect of Different Forms of Corrosion on Copper in Disposal Conditions**
  Martin Bojinov, Petri Kinnunen, Timo Laitinen, Christina Lilja, Kari Mäkelä and Timo Saario
- **Canister Fabrication and Emplacement Issues Related to Isolation**
  Daniel Bullen and Michael Apted
- **Analyzes of Coupled Heat and Moisture Flow in Unsaturated and Saturated Bentonite**
  Johan Claesson
- **Corrosion Experiments on Copper in Different Groundwaters**
  Hans-Peter Hermansson
- **Models for creep and creep fracture in copper**
  Kjell Pettersson
- **DECOVALEX Simulations Results Related to EBS**
  Jonny Rutqvist
- **The Potential Impact of the Presence of Concrete upon the Performance of the KBS-3 Design**
  David Savage
- **Simulation of Coupled T-H-M Processes in Engineering Barrier System For Disposal of Radioactive Waste and Spent Nuclear Fuel – A Review of DECOVALEX Project**
  Ove Stephansson
- **Interaction Between the Buffer Material and the Canister - Preliminary Analysis of Geotechnical Aspects**
  Göran Sällfors and Sadek Baker
- **A Summary of Key Technical Issues Related to Integrity of Engineered Barrier System**
  Chin-Fu Tsang

# ENRESA-FEBEX AND MOCK-UP TESTS

# LESSONS LEARNED AND OUTSTANDING ISSUES

Eduardo Alonso. *Professor of Geotechnical Engineering. UPC, Barcelona*

## 1. INTRODUCTION

The primary objective of FEBEX in situ test was to demonstrate the feasibility of a storage concept in an environment close to design conditions. Two additional objectives were specified: the test should serve also the purpose of checking the ability of current thermohydromechanical (THM) and thermohydrochemical models to perform accurate predictions. This note refers to one of these objectives: An assessment of the capability of making accurate THM predictions in view of the gained experience will be given. FEBEX in situ test was complemented with a parallel test (mock-up test), which was designed for redundancy and with a more scientific purpose in mind since boundary and initial conditions could be established with greater accuracy. The layout of the mock-up corresponds essentially to a smaller scale version of the in situ test. The link of this work with Performance Assessment issues is primarily related to the question of gaining confidence in predictive models. In FEBEX, the following sequence of activities leading to a proper model development was followed: materials involved (and specifically compacted bentonite) were fully characterised by means of laboratory tests, the site was thoroughly investigated, blind predictions of the numerical model were produced and they were later compared with field records of measured behaviour. However, the process of updating material properties on the basis of new and improved laboratory tests has been a continuous activity. Also, models used in first prediction exercises have evolved in the course of the test history. In a final development, currently in progress, a partial dismantling is providing new experimental data, which may be analysed and compared with predictions.

## 2. MEASUREMENTS VERSUS COMPUTATIONS. AN UPDATE

Computations have been performed with the finite element program CODE_BRIGHT (1,2). A number of reports, papers and doctoral thesis (3-8) cover the performance of laboratory tests and the determination of model parameters. A general overview of both tests, in situ conditions, material properties and model predictions is given in (9). Model predictions here correspond to a “base case”. Sensitivity analyses were also performed, although they will not be discussed here (see, however, 10).

## 2.1 In situ test

Temperature distributions were in general well predicted. Of particular relevance was the distribution and time development of relative humidity of the bentonite barrier. An example showing the comparison of model predictions and sensor data is given in Figure 1. It covers 1600 days of test operation.

Some concern was given to the apparent decrease in RH values in points close to the granite-bentonite boundary. However, they may be due to faulty sensor behaviour. Stresses are more difficult to predict (and to measure). This is shown in a similar comparison plot in Figure 2.

## 2.2 Mock-up test

Total water inflow can be measured in this test. Initial predictions were closely followed by measurements. However a significant and consistent departure was observed beyond the first year of operation. Considerable attention has been paid to this departure (Fig. 3). This slow-down of hydration (as compared with predictions) is also reflected in relative humidity, especially in buffer regions directly affected by strong temperature gradients (Fig. 4). Extension of predictions to long-term behaviour shows an asymptotic behaviour towards full saturation (which is theoretically achieved in around 5000 days). However, (Fig. 5), it is not clear that the test will behave in this manner.

# 3. THM MODELLING. RECENT DEVELOPMENTS

An explanation to the reduction of observed rates of hydration, if compared with predictions based on accepted theories, has been investigated through a number of alternative possibilities:

a) Modifying the water retention properties of the buffer. Available tests may be used to define the influence of temperature and porosity, which were not included in the initial formulations.

b) The intrinsic permeability was made dependent of current porosity.

c) Assumed boundary conditions were changed in an effort to explain the measurements. They were apparently consistent with the development of an impervious outer boundary in a cylindrical area directly affected by the heaters.

d) A threshold gradient in Darcy law was introduced.

e) A more sophisticated model to account for changes in bentonite microfabric was introduced. It may account for a reduction in permeability as the material expands.

Issues (a) and (b) were shown to have a limited effect. Regarding point (c), there are no indications of conduit clogging or malfunctioning of the hydration system. The remaining two possibilities, which are  focused on material behaviour will be briefly covered.

### 3.1 Threshold gradient

An examination of hydraulic gradients in a bentonite barrier during hydration reveals that the actual values are extremely high if compared with typical applications in geotechnical engineering (Fig. 6). In fact, due to the high suction values, calculated gradients in reported laboratory tests are, in general, higher than a few thousands. It is therefore difficult to obtain direct experimental evidence on flow at low gradients and one may speculate with a modification of Darcy's law in the sense that the flow is restricted or impeded below a given threshold gradient $i_o$. The implication of such a hydraulic model is shown in Fig. 7. In terms of the computed evolution of the relative humidity in Sections 4 and 10 of the mock-up test, long-term predictions show now that saturation will never be reached. Note that this prediction is consistent with the early known history of the test.

### 3.2 Evolution of microfabric

The representation of the compacted clay fabric as a double structure solid is a powerful tool to describe specific features of expansive materials both from a mechanical and from a hydraulic point of view. Several papers developing this idea have been published (11-13). The total void ratio is, in these models, made of two additive terms: the macro and the micro void ratios. Both evolve and interact as the material is wetted (or dried). The observable permeability is fundamentally linked to the macroporosity. If the mechanical constitutive model is capable of describing the evolution of porosities, then a model for the evolving permeability is derived.

These ideas were also implemented in CODE_BRIGHT which was then used to model the mock-up test. Some results are given in Figures 8 and 9. The known history of water intake and relative humidity changes is well reproduced by this model. Note that the model predicts a full hydration of the barrier at some time (unlike the threshold gradient model whose predictions are also shown in Figures 8 and 9). This is an unfortunate situation since alternative models, which are based on plausible physical phenomena and are capable of matching the early transient history of the tests, exhibit different long-term behaviour

## 4. SOME PRELIMINARY RESULTS FROM DISMANTLING

The first heater area and the surrounding bentonite buffer were excavated, layer by layer. A radial pattern of extracted samples, at close locations, allows the representation of contours of dry density and water content. These values could be readily determined at the site, immediately after sampling. The variation of both variables in a section affected by the heater is shown in Figure 10. As expected, the water content follows a strong gradient from the dry inner regions to the wet outer layers. More interesting is the distribution of dry densities. The outer rings have expanded, whereas the inner ones have shrunk. Figure 11 shows the interpolated pattern of dry densities. It is unlikely that the full hydration of the barrier will restore the initial (constant) distribution of block's dry densities. This is due to the well documented stress-suction path dependent of bentonite.

Laboratory experiments show this behaviour (Fig. 12). Samples shown in this plot (S2, S3, S4) were tested in a suction controlled oedometer cell capable of handling high suction and stress changes. Sample S4 may be representative of a point of the outer ring: it is initially wetted and then loaded. Sample S2 is more representative of an inner ring, close to the heater: it is initially dried and then loaded. However, the samples are finally taken to a wet state (under load) so that the final stress point is common to all of them. Note that the accumulated strains are different. Samples initially wetted remain at a higher void ratio.

The implications for the barrier performance are that a variable bentonite density profile will be reached in the long-term with a more porous material close to the rock and a denser material in the vicinity of the canister.

## 5. CONCLUSIONS

A number of conclusions may be derived from the observed behaviour of FEBEX experiments:

- Current THM modelling of in situ test, using the best available information of material properties reproduce in a satisfactory way the known history of buffer behaviour (for a period of 1600 days).
- Deviations from predictions of measured water input, relative humidities and stresses of the parallel mock-up test is, in general terms, explained by a reduction of expected hydration rates.
- Some possible reasons for the decrease in the hydration rate have been explored. The presence of a threshold gradient in the formulation of the Darcy equation or the progressive decrease of intrinsic permeability of the buffer due to changes in microstructure may explain the observed behaviour. However, they lead to different long-term predictions. In particular, a threshold gradient implies that full saturation will not be achieved, an issue of direct relevance to Performance Assessment. Short-term tests do not provide the necessary data to settle this question. More refined testing techniques or field observations in the medium term may give information to favour one hypothesis over alternative ones.
- The process of buffer hydration and transient dessication probably leads to a permanent heterogeneous distribution of barrier density (and therefore of water content) in the long term.

## ACKNOWLEDGEMENTS

The author acknowledges the contribution and support of his colleagues, A. Gens, A. Lloret and M. Sánchez in the preparation of this paper.

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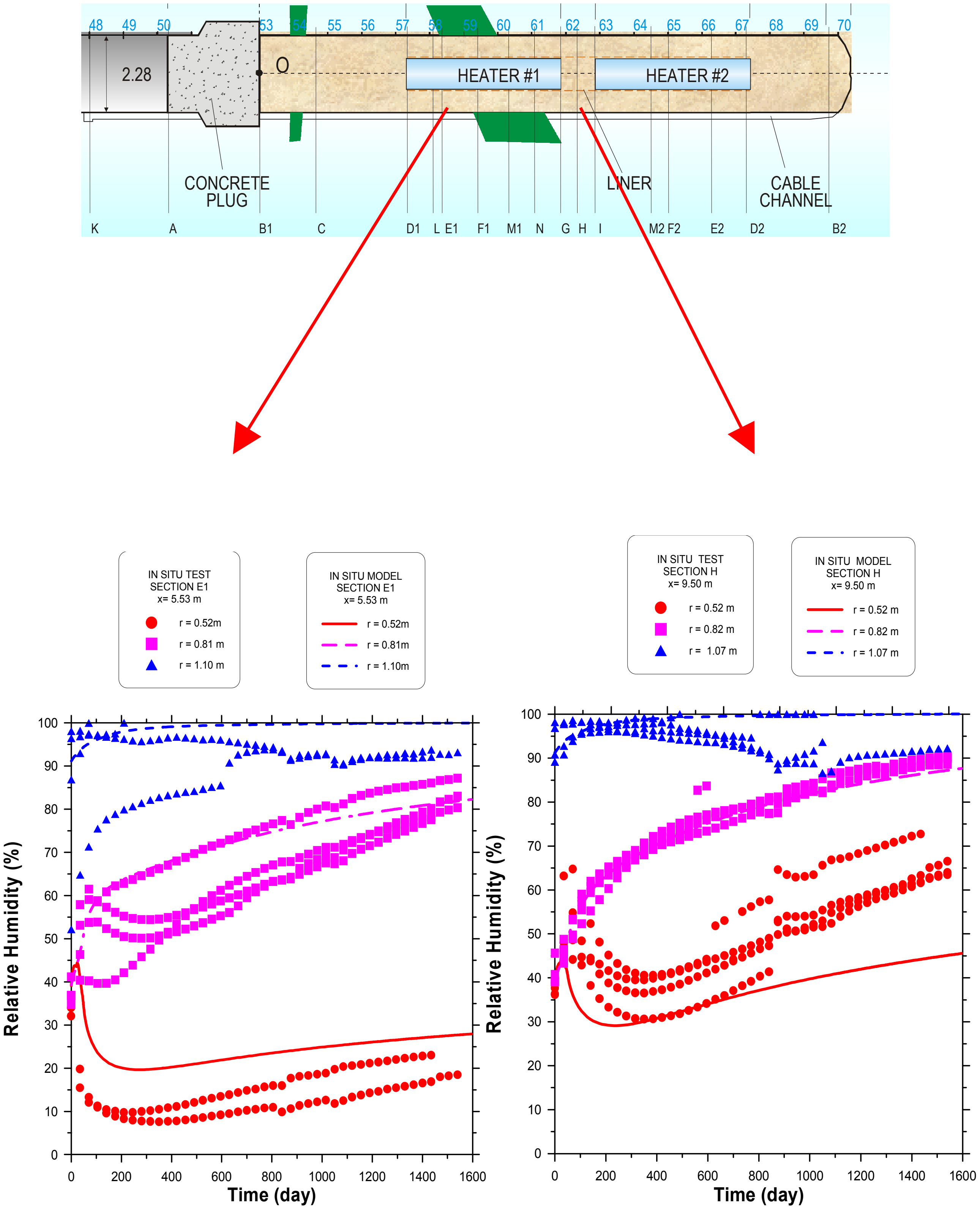


Figure 1: In situ test. Comparison of measured histories of relative humidity ad model predictions.

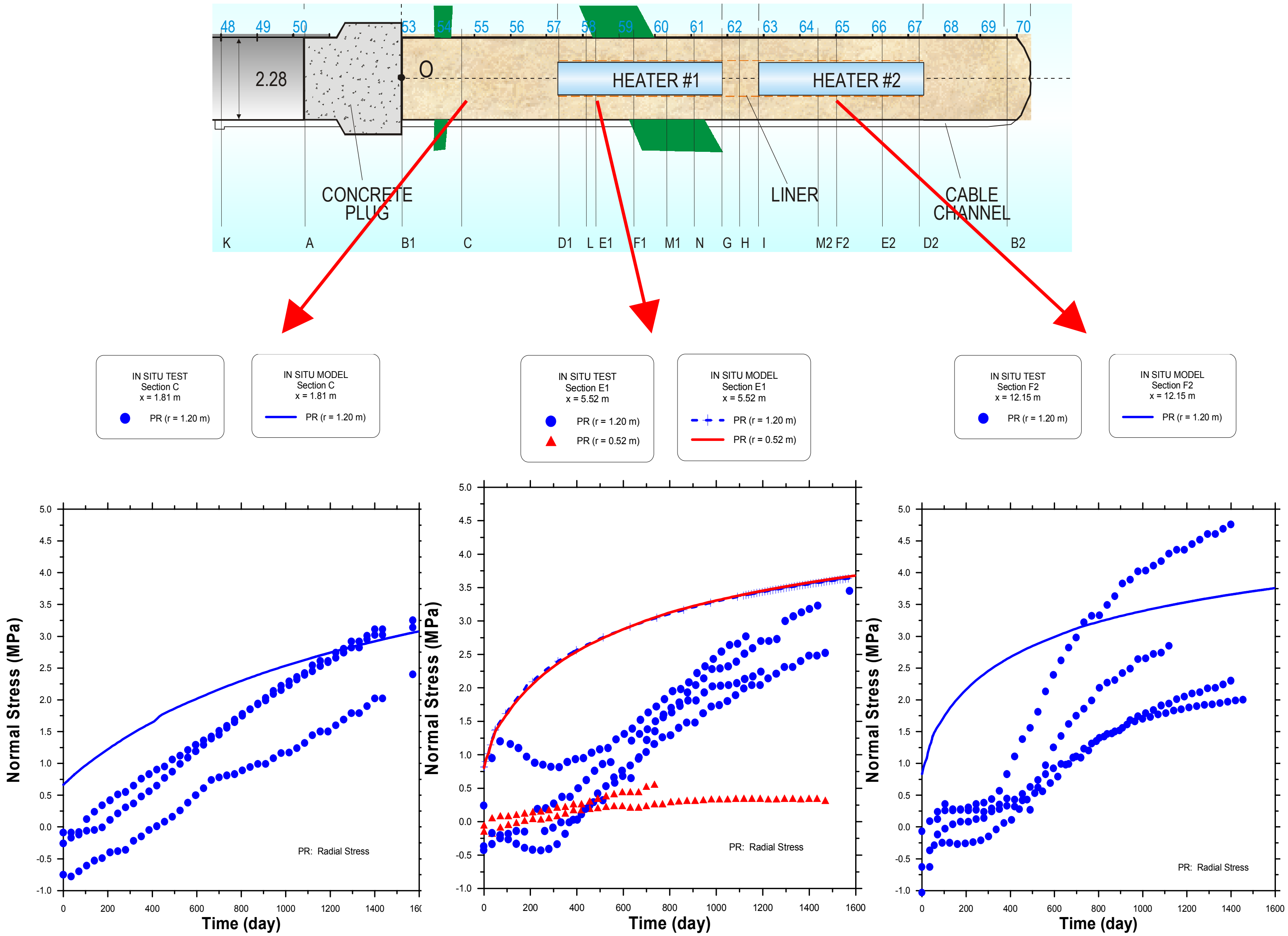


Figure 2: In situ test. Comparison of measured histories of radial stresses and model predictions.

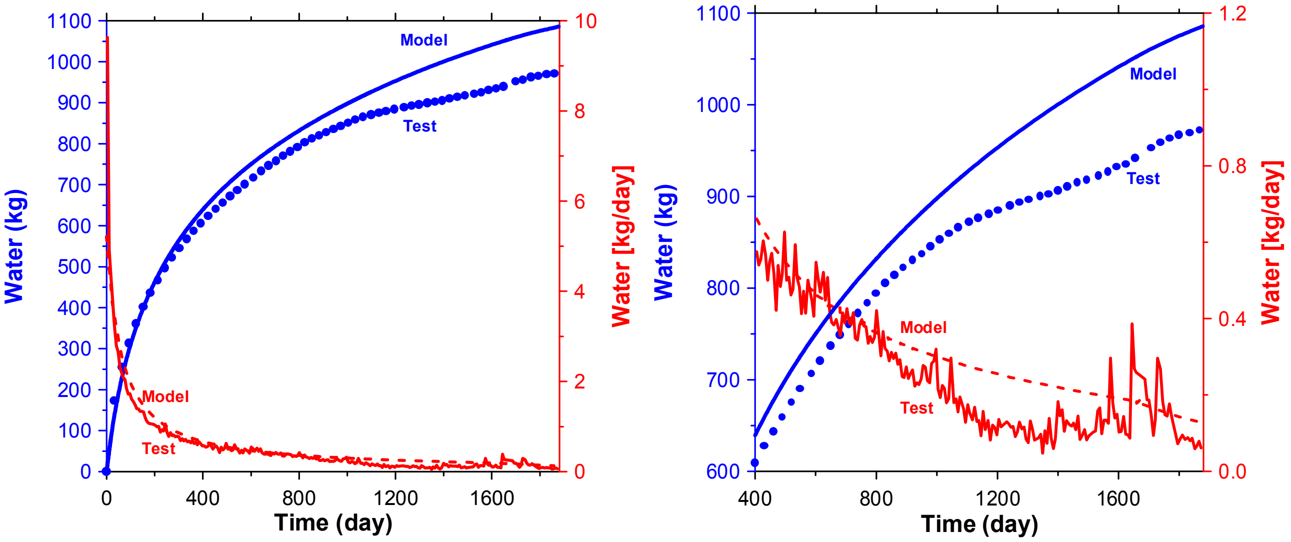


Figure 3: Mock-up test. Comparison of measured evolution of water inflow and model predictions.

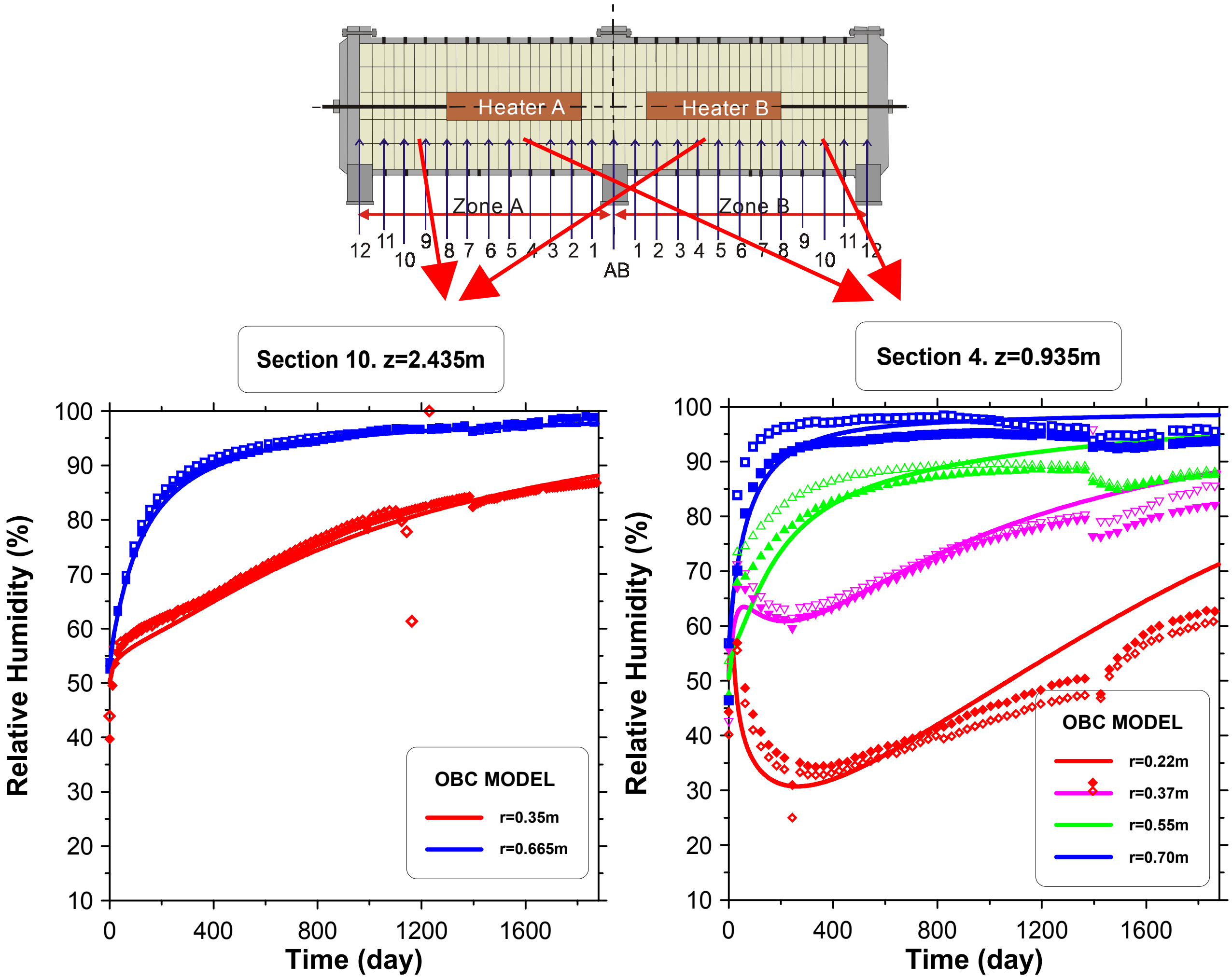


Figure 4: Mock-up test. Comparison of measured evolution of relative humidity and model predictions.

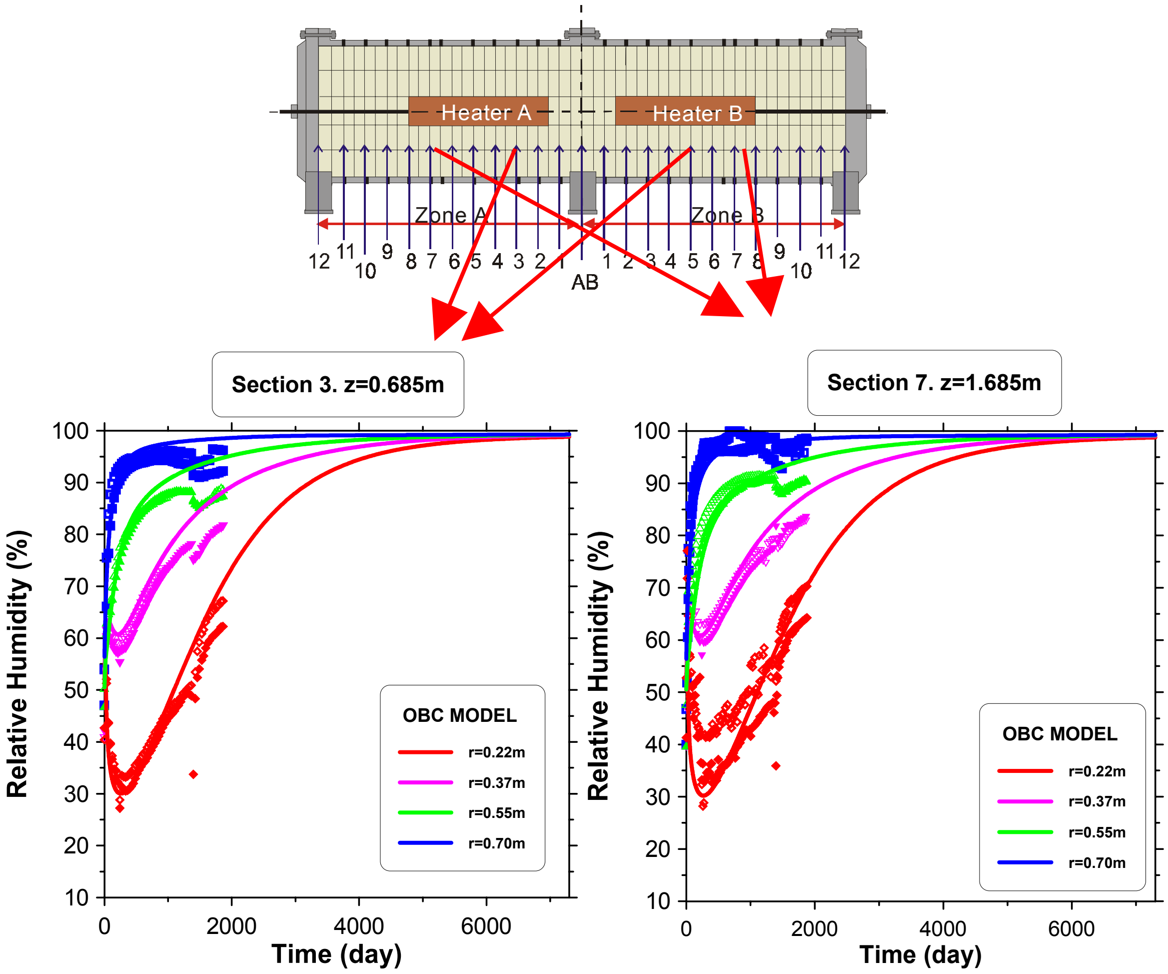


Figure 5: Mock-up test. Long-term predictions of relative humidity.

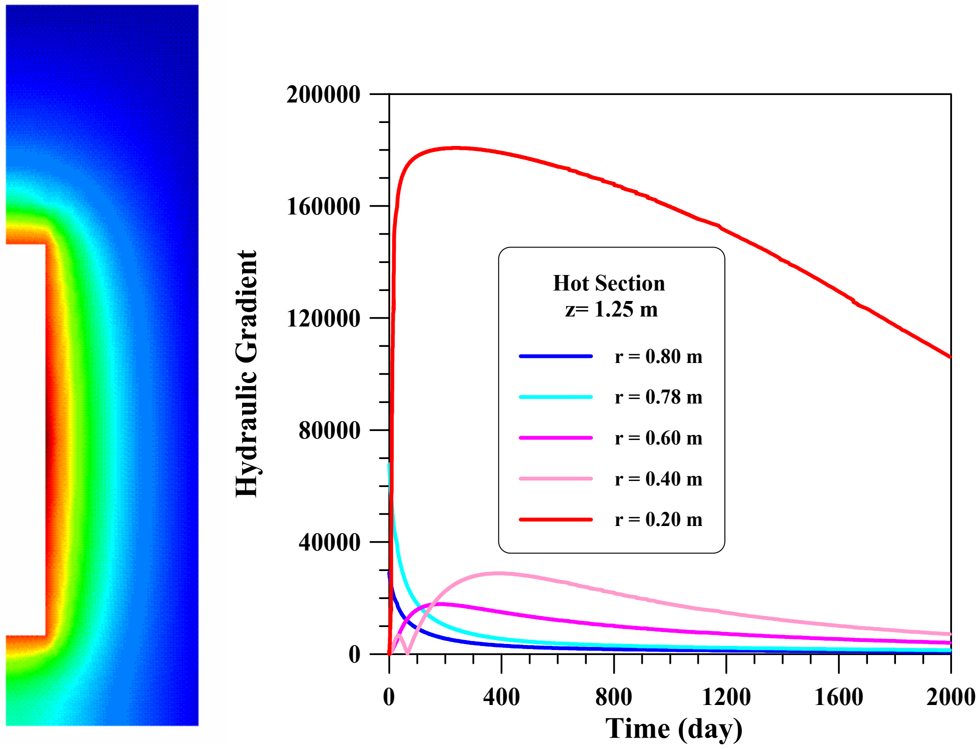


Figure 6: Mock-up test. Derived flow gradient in radial direction.

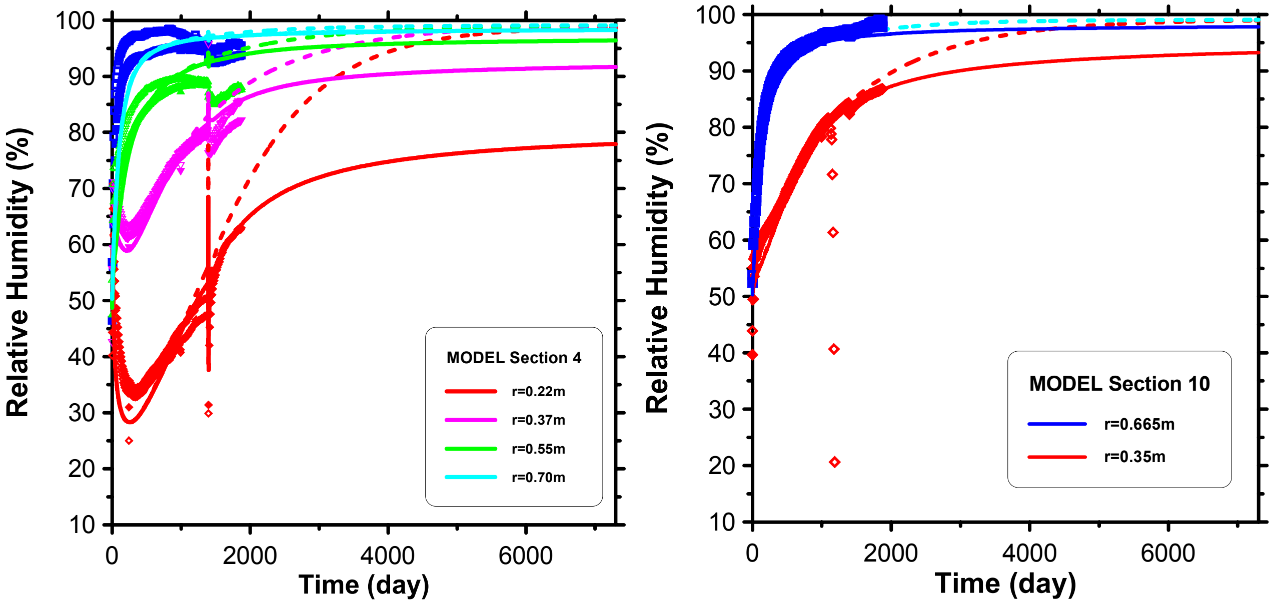


Figure 7: Effect of threshold gradient in RH calculations in Sections 4 and 10 of mock-up test.

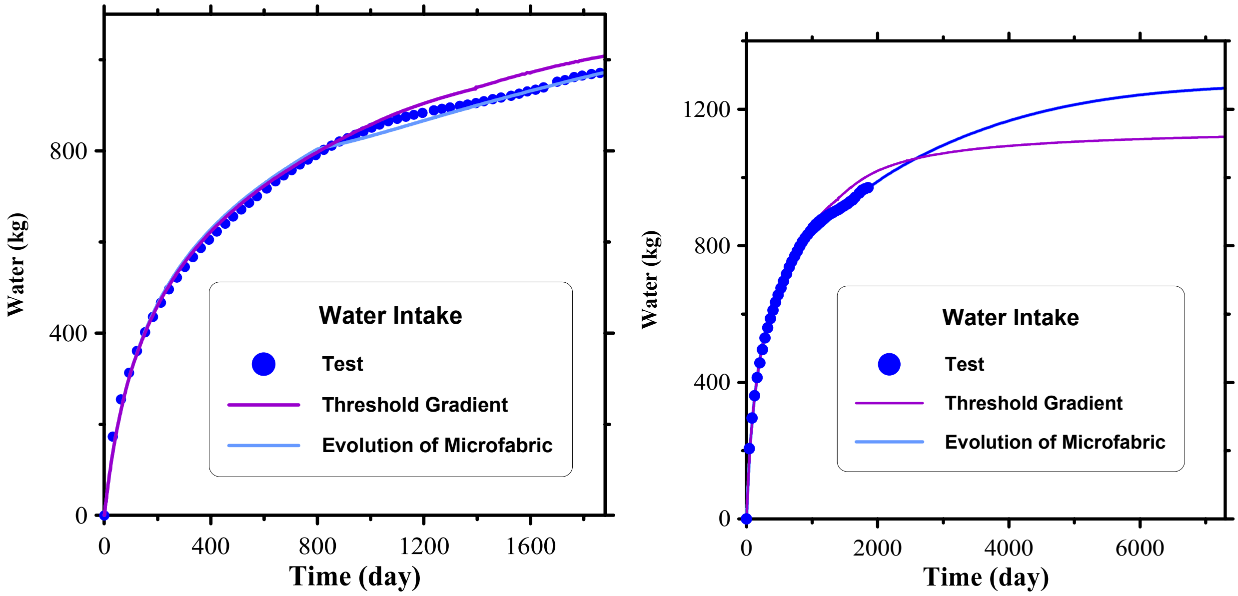
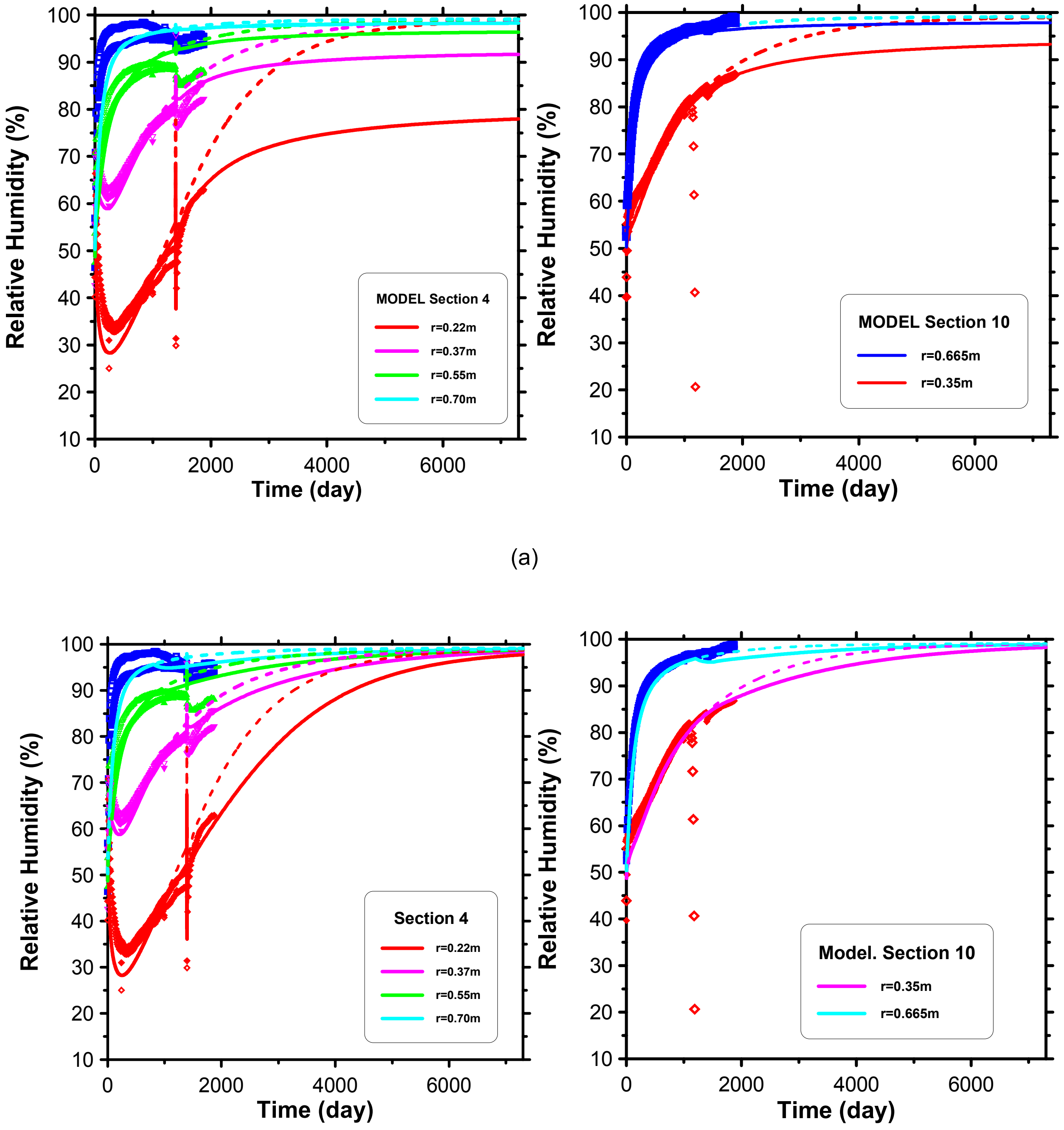


Figure 8: Mock-up test. Long-term predictions of water intake.



(a)

(b)

Figure 9: Mock-up test. Evolution of relative humidities in Section 4 and 10 of mock-up test. (a) Threshold gradient and (b) evolution of microfabric.

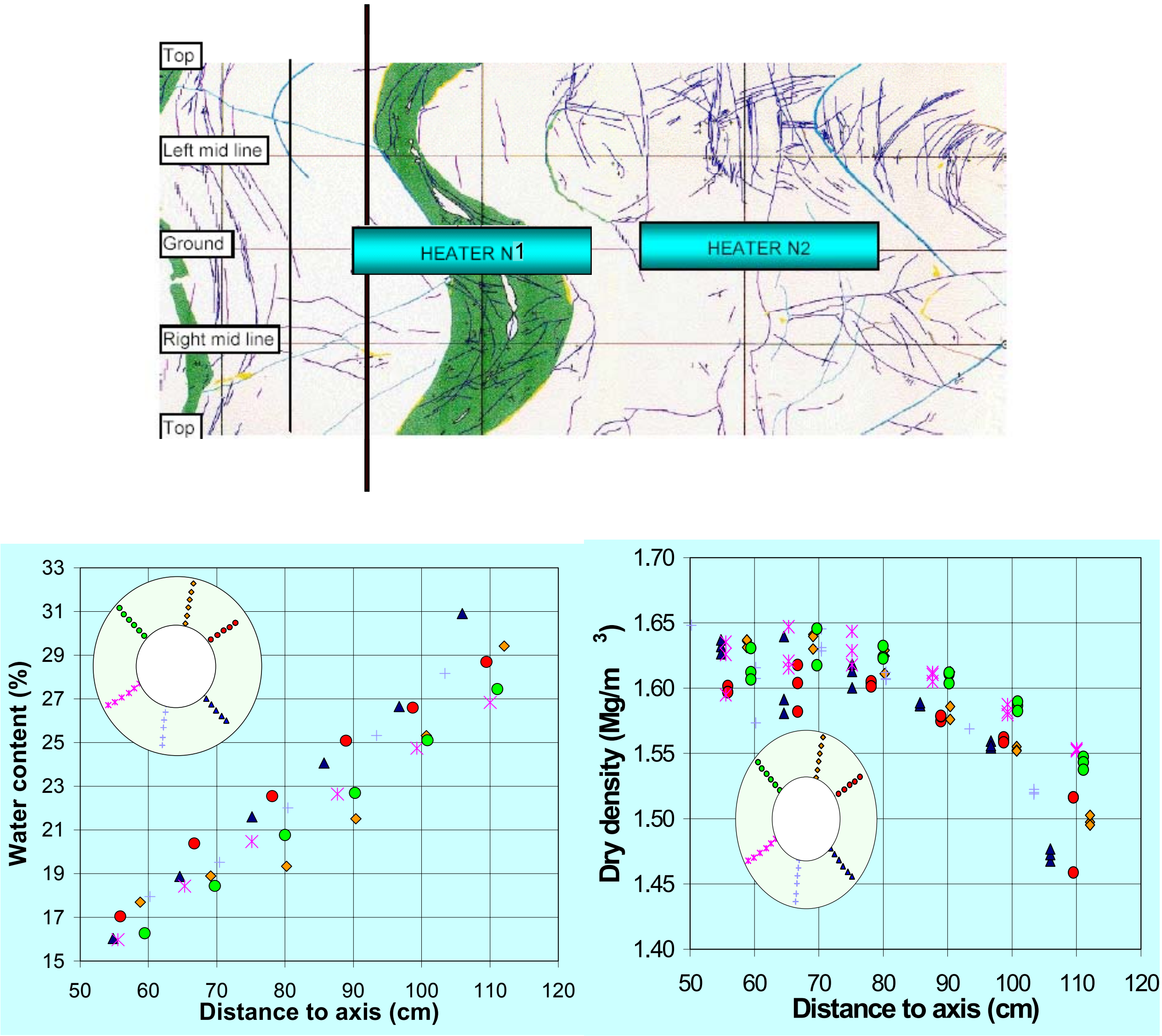


Figure 10: Dismantling FEBEX in situ test. Measured distributions of water content and dry densities in Section 18.

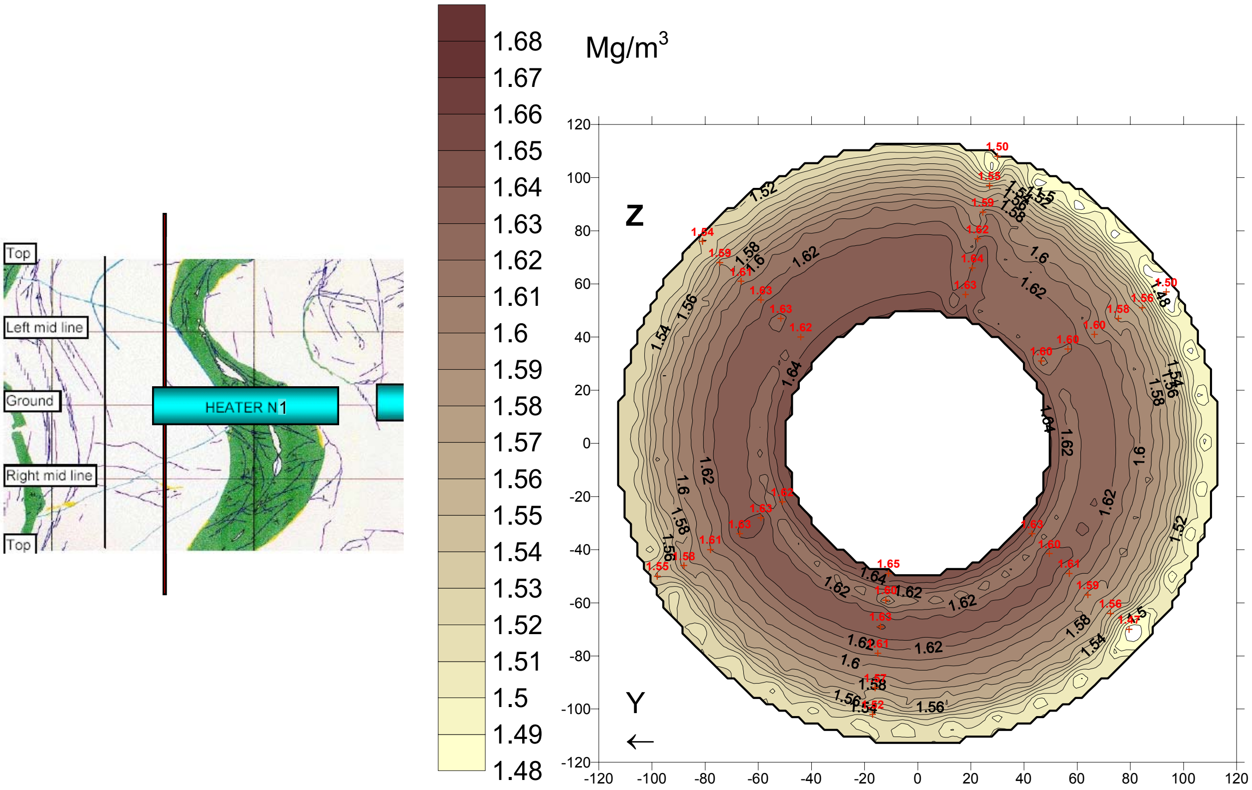


Figure 11: Dismantling of FEBEX in situ test. Interpolated contours of dry density of bentonite buffer in Section 18.

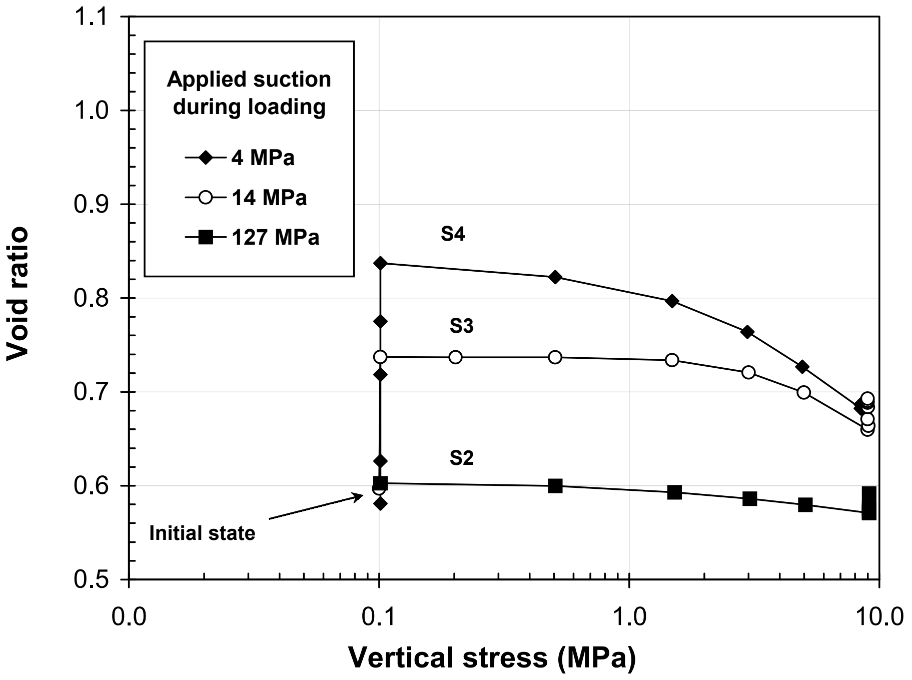


Figure 12: Variation of void ratio observed in tests S2, S3 and S4 with the same initial and final stress states.

# Development of coupled THMC models of buffer evolution

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## INTRODUCTION

The Swedish Nuclear Power Inspectorate is evaluating models of coupled thermal (T), hydraulic/transport (H) mechanical (M) and chemical (C) processes controlling the evolution of the near field in a KBS-3 repository for spent nuclear fuel. We have tested one such modeling approach in a preliminary evaluation of whether the bentonite buffer could experience significant cementation resulting from irreversible mass transfer among buffer minerals and pore fluids during the early non-isothermal phase of repository evolution [1]. The present paper briefly summarizes the results of that study, and discusses work currently underway that is designed to further evaluate whether the basic modeling approach can be extended to more realistic models of buffer evolution.

## MODEL DESCRIPTION

The model system is based on the KBS-3 disposal concept and thus consists of a cylindrical shell of water-saturated bentonite, 35 cm thick, located between the canister and host rock. A one-dimensional radial coordinate system is assumed, with a zero-flux boundary condition at the canister-buffer interface and an open boundary condition at the buffer-rock interface. Mass and energy cross the latter boundary, and solute concentrations at this boundary are thus assumed to change with time. Solute concentrations in the host rock are fixed, however, and thus determine Dirichlet boundary conditions to the governing reactive-transport equations.

The initial state of the system is perturbed as the temperature inside the buffer begins to rise. It is assumed that the thermal evolution of the buffer follows that predicted for the KBS-3 near field [2]. The system is represented by a highly simplified set of reactions involving two common accessory minerals of bentonite, calcite and quartz, and their corresponding aqueous species. The rates of the aqueous reactions are assumed to be instantaneous, but the rates of heterogeneous reactions involving the minerals are assumed to be kinetically controlled. These two minerals were selected for initial analysis because the solubility of quartz is prograde (thus increasing with increasing temperature), whereas that of calcite is retrograde (decreasing with increasing temperature). To further simplify the model, it is assumed that the volume fractions of these two minerals are equivalent (35%), and equal to one half the total solid volume of the buffer.

We model this system using an object-oriented programming technique and a sequential iterative approach to solve the coupled system of partial differential equations and differential algebraic equations describing system evolution. The mass conservation equations include both transport and temperature-dependent reaction terms:

$$\frac{\partial(\phi C_i)}{\partial t} - \nabla \cdot (D\phi\nabla C_i) = \sum_{j=1}^{N_r} \nu_{ij} R_j \qquad i = 1,\ldots,N_C. \tag{1}$$

where $C_i$ denotes the aqueous concentration for the $i$-th species [mol/l], $D$ stands for the diffusion coefficient ($m^2/s$; diffusion is the only relevant transport mechanism in the buffer), $\phi$ refers to porosity, $\nu_i$ denotes a stoichiometric coefficient for the $i$-th species in the $j$-th reaction, and $N_C$ stands for the number of aqueous species in the system. For minerals, the transport term is absent, and the mass conservation equation then takes the following form [3]:

$$\frac{\partial \phi_m}{\partial t} = \overline{V}_m R_m \qquad m = 1,\ldots,N_m, \tag{2}$$

where $\phi_m$ denotes volume fraction, $\overline{V}_m$ refers to molar volume [$m^3$/mol], $R_m$ represents the dissolution/precipitation rate for the $m$-th mineral [mol/s], and $N_m$ stands for the number of minerals. Solutions to the system of Eqns. (1) and (2) are obtained using the general solver PETSc (Portable and Extensible Toolkit for Scientific computing; [4]).

## PRELIMINARY RESULTS AND DISCUSSION

Cementation is potentially a concern because it could alter the swelling pressure, deformability, thermal conductivity and hydraulic conductivity of the buffer, and thus possibly affect adversely the primary isolation functions of this EBS component to protect the canister from movements in the near-field rock and to provide a stable diffusional transport pathway between the rock and canister. Although the mechanisms involved in these physical and rheological consequences of buffer cementation are poorly understood at this time, it is reasonable to assume that they must correlate in some meaningful way with net changes in porosity resulting from mineral dissolution and precipitation. On the basis of this qualitative correlation and calculated results using the model described above, it appears that the extent of buffer cementation may be minimal for conditions expected in the KBS-3 near field.

Support for this conclusion is given in Fig. 1a, which shows calculated variations in the volume fractions of quartz and calcite, and resultant changes in porosity, at the canister-buffer interface during the first 100,000 years of repository evolution (corresponding to the maximum duration of the thermal pulse resulting from the release of decay heat from spent fuel). As can be seen, the change in volume fraction of both minerals is negligible during this period, and this results in similarly negligible changes in porosity. The conclusion is also supported by calculated spatial variations in mineral volume fractions and porosity corresponding to the time of maximum thermal gradients in the buffer (Fig. 1b). Model results suggest that a slight increase in volume associated with calcite precipitation at the hot end of the buffer is almost exactly balanced by a slight decrease in volume resulting from quartz dissolution. The net change in mineral volume is negligible

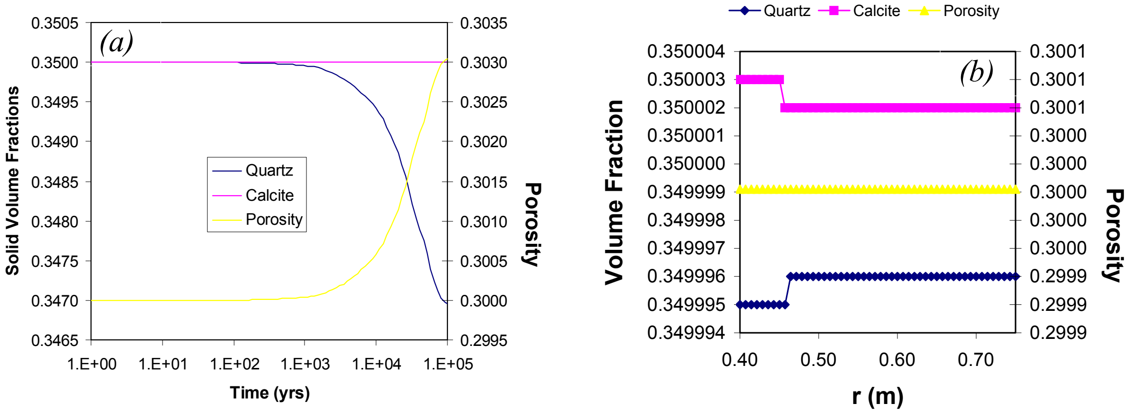

*Figure 1. Temporal variations in buffer porosity and mineral volume fractions at the canister-buffer interface (a), and spatial profiles of porosity and mineral volume fractions after 100 years (b) [canister-buffer boundary at r = 0.4 m and buffer-rock boundary at r = 0.75 m].*

and the porosity is therefore essentially unchanged.

These results seemingly conflict with the results of field, experimental, modeling and natural-analogue studies [*e.g.,* 5 - 7], which indicate that the mineralogy and associated rheological properties of bentonite and other argillaceous materials are indeed strongly affected by heating. The temperatures and temperature gradients considered in these other studies are significantly greater than those that are relevant to the KBS-3 near field, however. The lower temperatures and much smaller temperature gradients in the near field appear to be insufficient to generate any appreciable cementation of the buffer.

Our results are preliminary and substantial modeling improvements are clearly needed before a more definitive statement can be made regarding the potential for significant buffer cementation in the KBS-3 near field. It should be noted in this regard that more sophisticated chemical models of buffer cementation have already been developed using similar modeling techniques [8]. However, these alternative models apparently do not account for coupled processes arising from the effects of changes in porosity on the diffusional transport velocity of aqueous solutes and rates of mineral-fluid reactions. We believe it is essential to include such couplings in models of buffer cementation because changes in porosity and pore structure are correlated with changes in the mechanical and rheological properties of the buffer [9]. It is these latter properties that are important because they determine whether the isolation requirements of the buffer can be met.

We believe that the main conclusion from our preliminary work is that the basic, object-oriented modeling approach appears to be sufficiently robust that it can be extended to include more realistic geochemical models of bentonite-porewater interactions. The model that is presently being evaluated includes both time- and temperature-dependent reactions controlling the dissolution/precipitation and ion exchange behavior of smectite, which is the dominant mineral constituent of the buffer. The accuracy of the revised model will be evaluated based on the results of relevant field and experimental systems at high temperatures. The potential for buffer cementation will then be re-assessed using the more realistic model under relevant near-field conditions. Associated impacts on the physical and mechanical properties of the buffer will be qualitatively assessed based on calculated changes in the buffer's porosity.

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# Creep and creep damage in copper under uniaxial/multiaxial loading

## Abstract

Multiaxial tensile loading is known to enhance accumulation of creep cavitation and cracking damage in polycrystalline metals under given equivalent loading stress and temperature (Fig 1). To study whether this could potentially lead to significant creep damage under long-term repository conditions, multiaxial creep testing and damage evaluation has been initiated.

Multiaxial creep testing of OFP copper has been performed using sharp notches in compact tension (CT) specimens. The loading conditions (reference stress and temperature) have been selected to produce an estimated time to either failure or at least to measurable creep damage within the maximum intended testing time or about 5000 hours. For appropriate material and finite element (FE) modelling to set correct loading in multiaxial testing and to obtain a reasonable stress state conversion, parallel uniaxial creep testing has also been performed on the same material.

In addition, to support the uniaxial testing and materials modelling, an overall creep rupture life assessment was performed for OFP copper, based on ECCC guidelines and PD6605 including uniaxial creep testing data from the literature.

To observe potential creep damage, the multiaxial tests have been also interrupted for metallography about every 2000 h of testing, and inspected by scanning electron microscopy (SEM) for indications of damage. For comparison, metallographic inspection including transmission electron microscopy (TEM) was performed for the same material in as-new state.

The initial as-new state as well as later tested states of the material appear to involve grain boundary phases, which are sometimes apparent in SEM but can also require TEM to be resolved (Fig 2). Until now, the multiaxial creep test at lowest reference stress (46 MPa / 150°C) has been interrupted at 3000, 5000 and 7000 h of testing for inspection in SEM. In these inspections, only occasional scattered evidence of some possible cavitation damage has been found so far (Fig 3). On the other hand, the difference in the time scales of testing (10 000 hours) and the application (about 100 000 years) is very large. The difference remains extensive even when the application is compared with usual engineering structures having a design life of some 30 to 100 years, requiring creep testing up to about 100 000 hours (about 11.5 years).

That long-term testing is indispensable for reasonable creep life prediction, was also evident from the available uniaxial creep rupture data. These do not give as yet reliable evidence even for the conventional engineering range of design life. It is therefore suggested that testing is continued to provide improved confidence on the trends in creep strength at low stresses and temperatures.

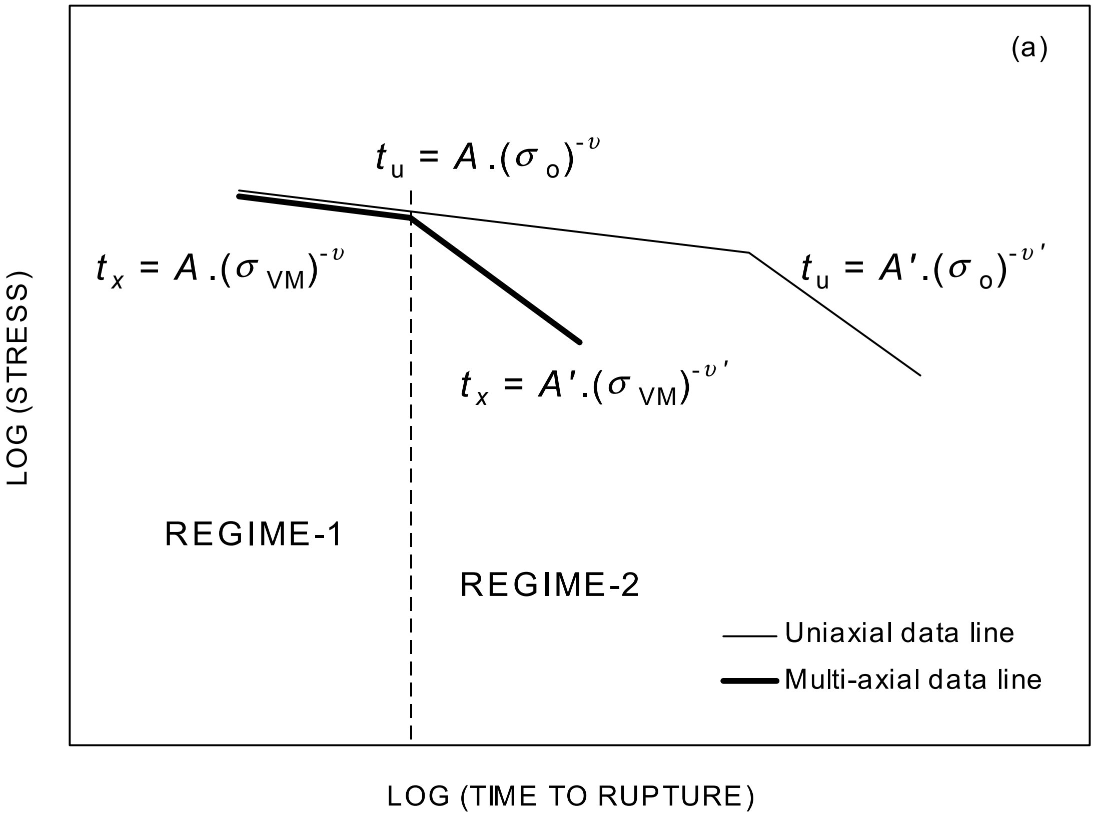

*Fig 1. The principle of creep damage acceleration due to multiaxial creep loading.*

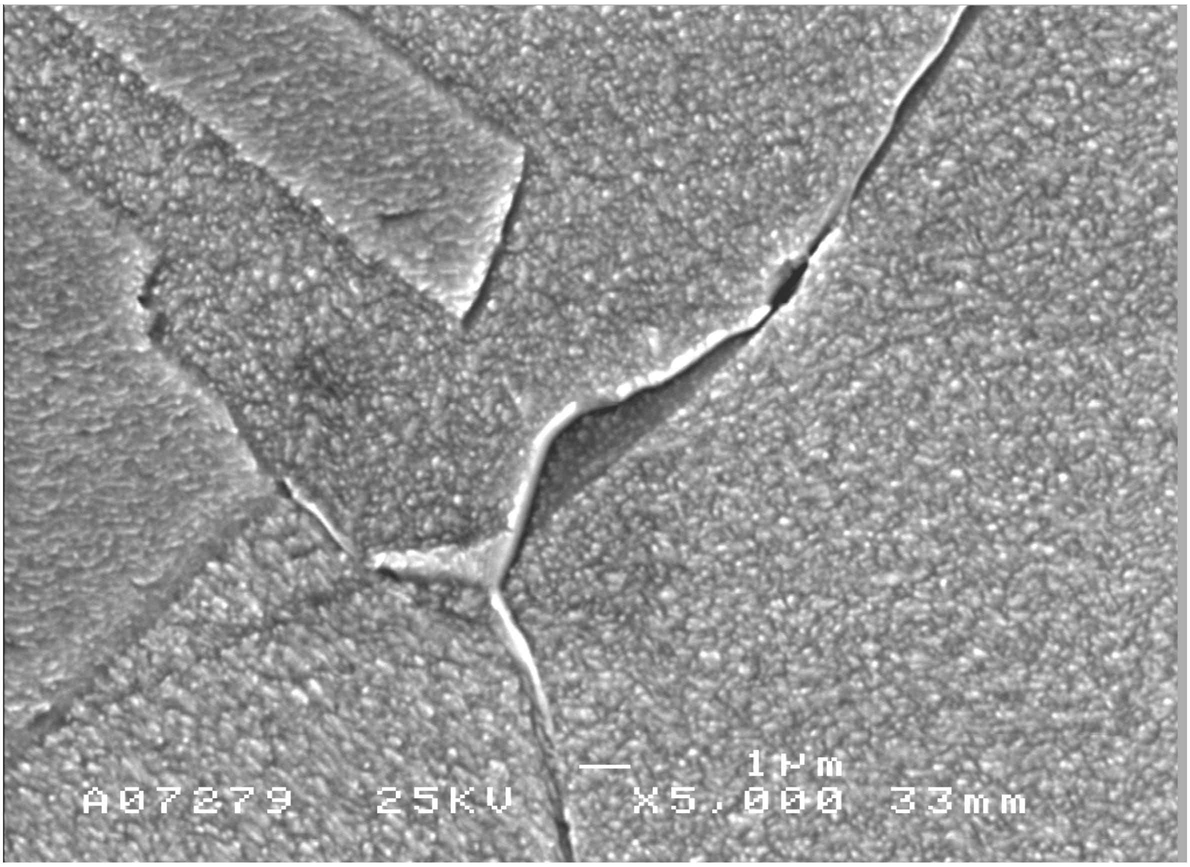

*Fig 2. The notch tip region with a grain boundary phase, after 5000 h of testing (46 MPa/150℃).*

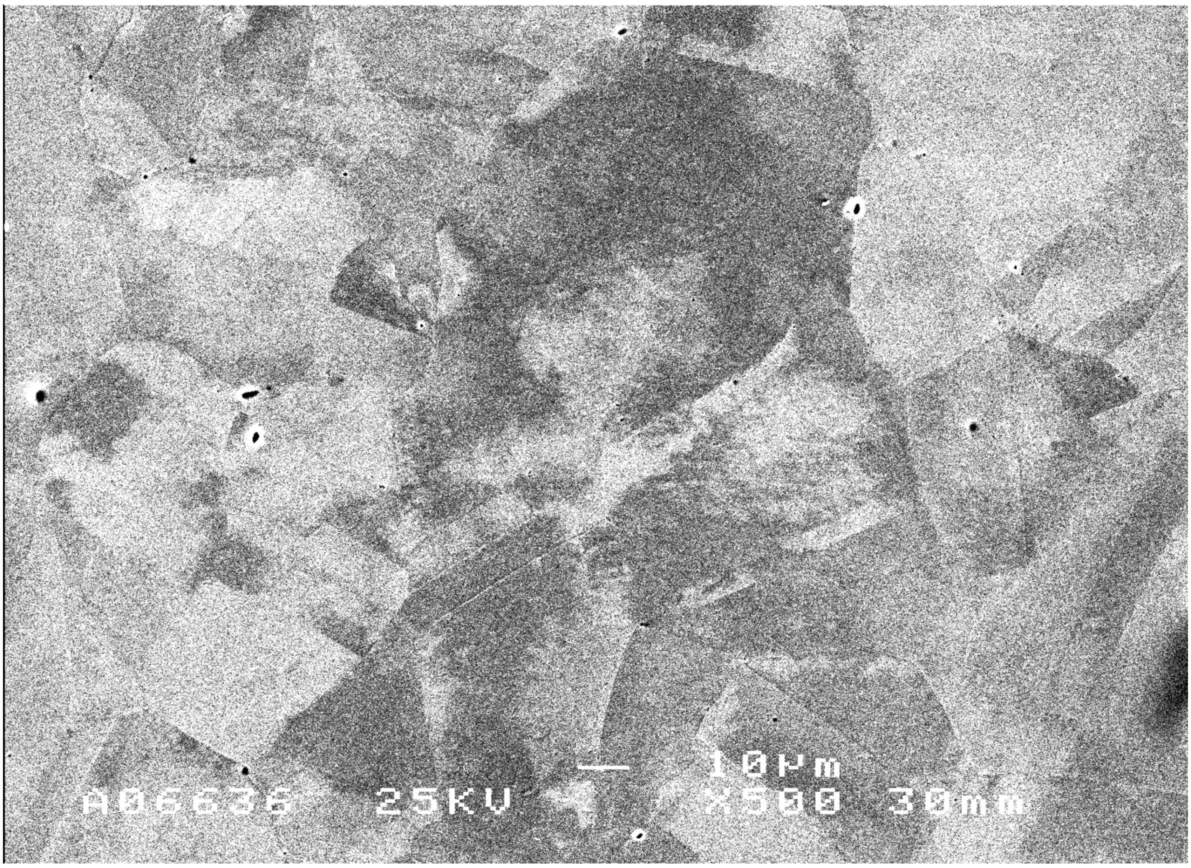

*Fig 3. Notch tip region in the side surface of CT specimen, after 3000 h at 46 MPa/150°C.*

# THE EFFECT OF DIFFERENT FORMS OF CORROSION ON COPPER IN DISPOSAL CONDITIONS

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To assess the corrosion resistance of the copper shield, three major corrosion types are considered in this paper, namely stress corrosion cracking, pitting corrosion and general corrosion. The approach presented in this paper is based on assessing whether the occurrence of different types of corrosion can be excluded in the disposal conditions. If this is not the case, we recommend to predict the maximum corrosion penetration on the basis of experimental results and to assess, if it is below an acceptable level. We have applied this approach to show that the occurrence of stress corrosion cracking in the presence of nitrite ions in the disposal conditions can very likely be excluded. We have also shown that assessing the occurrence of localised corrosion due to bicarbonate ions and the occurrence of general corrosion in the disposal conditions requires further experimental work.

## 1. DISPOSAL CONDITIONS

The pressure in the final disposal vault consists of two components, the hydrostatic pressure of the water (7 MPa at 700 m depth) and the swelling pressure from the bentonite (up to 7 MPa). The total pressure estimated to prevail at the copper canister surface is then a maximum of 14 MPa.

During the transient phase immediately after the closure of the repository the conditions will be first oxidising, after which reducing conditions will gradually be re-established. The undisturbed natural redox conditions of the groundwater at depth of all the Finnish investigation sites including Olkiluoto and Hästholmen sites have been estimated to result in redox potentials in the range -0.2 $V_{SHE}$ ... -0.3 $V_{SHE}$, (at ambient temperature) depending on the pH (e.g. Anttila et al. 1999a). The canisters reach their maximum temperature of about 90 °C in the repository within 20 years after the disposal, after which the temperature will slowly decrease towards the temperature of the surrounding bedrock.

At some sites chloride ions have been found in the groundwater up to a concentration of 40000 mg/l close to the planned depth of the repository. In the analysis of the groundwater composition in Finland and Sweden small amounts of ammonium ions ($NH_4^+$) have been found. The maximum concentrations have been about 3 mg/l at the Hästholmen site and 1.1 mg/l at the Olkiluoto site (Anttila et al. 1999a, 1999b), but otherwise ammonium ions have been mainly found in the upper part of the bedrock (100-200 m depth). Ammonium ions, as well as nitrite ions, nitrate ions and acetate ions, are known to make copper prone to stress corrosion cracking. The nitrite and nitrate ion concentrations in some single samples from Olkiluoto and Hästholmen sites have been 0.01 mg/l $NO_2^-$ and 0.03-0.3 mg/l $NO_3^-$. Mostly nitrite and nitrate ion concentrations are below detection limits (0.01 mg/l), as would be expected in deep reducing groundwater and the reported analytical results are associated with uncertainties due to analytical problems. Acetogenic bacteria have been observed in the groundwater of the investigation sites, these may form acetate ions. Carbonate ions, which are known to make copper prone at least to pitting corrosion, have been found at Olkiluoto and Hästholmen sites in maximum concentrations of 250-400 mg/l in the upper part of the bedrock. In the saline water at the depth below about 500-600 m the corresponding concentrations have been found to be 20-50 mg/l.

## 2. STRESS CORROSION CRACKING AND CREEP

Considering the longevity of the corrosion resistance of the copper shield, the occurrence of stress corrosion cracking should be completely avoided. This is because once initiated, the cracking is likely to cause severe damage. Accordingly, the application of the exclusion principle when assessing the occurrence of stress corrosion cracking seems especially justified and attractive. Sufficient knowledge is on the other hand not yet available to assess the effect of multiaxial stress state and the effect of environment on creep. It is thus not yet possible to decide exactly what kind of approach should be chosen to assess the risk related to creep phenomena.

Effective stress levels are likely to be important from the viewpoint of both stress corrosion cracking and creep. The expected momentary maximum stress levels from e.g. canister handling would be normally of the order of 15 to 35 MPa (Raiko and Salo, 1999), but forced straining beyond yield could occur locally due to external pressure loads in the repository. The canister shell base material is in hot-formed condition and the electron beam (EB) welds are in cast condition. The yield strength of this kind of copper is about 50 MPa at room temperature and the ultimate strength more than 200 MPa.

The canisters reach their maximum temperature of about 90 °C in the repository within 20 years after the disposal. Now we presume that simultaneously when reaching the maximum temperature the canister overpack is deformed due to creep or plastic deformation under the external pressure load. As a result of these deformations the whole radial 1-mm gap between the cylindrical overpack and insert will be closed. Due to the possibly very slowly increasing external pressure load the copper overpack will be deformed until a full contact is reached on all surfaces between the overpack and the iron insert. According to earlier calculations, when the 1-mm radial gap between the overpack and the insert is forced to close the actual maximum local strain in the copper overpack will be about 2%. This 2% strain corresponds to a stress level of ca. 80 MPa in hot-formed copper (Raiko and Salo, 1999).

The local tensile stress component in the corner area of the copper shell thus exceeds the copper yield strength (50 MPa) on the surface. However, the stress distribution over the wall thickness is such that most of the wall thickness is in a compression state. In addition, these kind of residual stresses are displacement controlled; in other words, the residual stresses are relaxed, if cracking or creeping occurs.

Raiko et al. have suggested that the postulated cracking cannot penetrate the whole wall, because the crack growth is stopped when the tension stress is relaxed in the area and the crack front reaches the compressive stress area. In spite of possible local crack initiation and growth, the remaining wall thickness (more than half of the nominal wall) will be thick enough for the corrosion allowance. The possible combined effect of creep and stress corrosion cracking cannot be properly dealt with at the moment because of the lack of relevant creep data. On-going experimental work has indicated that a multiaxial stress state accelerates creep in copper markedly (unpublished work). The repository environment is expected to further accelerate creep. Therefore, experimental data on creep of copper under multiaxial stress state and in closely simulated repository conditions is needed to fully assess the effect of creep on lifetime of the copper shield.

We recommend as the next step according to the chosen approach to find out if the occurrence of stress corrosion cracking can be excluded in the chemical conditions of the waste repository environment. The chemical constituents known to be able to induce stress corrosion cracking in copper and to exist in the Scandinavian groundwater are nitrite, ammonium and acetate ions. In the two recent investigations of stress corrosion susceptibility of copper in simulated ground water conditions in the presence of ammonium ions (King et al., 1999; Arilahti et al., 2000) no sign of stress corrosion cracking has been found. In the case of acetate ions, more experimental data are needed in order to exclude the possibility of stress corrosion cracking (Saario et al., 1999). The case of nitrite ions is discussed in more detail below.

### *EXAMPLE OF THE EXCLUSION PRINCIPLE; NITRITE IONS*

Based on published results (Benjamin et al. 1988), nitrite ions do not cause SCC in copper at concentrations below 0.001 M, which is equal to 69 mg/l, or at potentials lower than +0.1 $V_{SHE}$ in slightly alkaline solutions. The reported concentration of nitrite ions in some groundwater samples at the Hästholmen and Olkiluoto sites have been 0.01 mg/l (associated with large uncertainties). This is roughly four decades lower than the concentration of 69 mg/l. Additionally, the potential which has to be exceeded for SCC of copper to occur in nitrite ion containing environment, +0.1 $V_{SHE}$, is high (a potential where Cu(II) can be formed is required), in comparison with the redox potentials (and thereby also corrosion potential of copper) measured and predicted to prevail in the ground water of the disposal vault environment. It seems thus clear that the occurrence of SCC of copper due to the effect of potentials and nitrite ions can be excluded in the conditions prevailing at the Hästholmen and Olkiluoto sites (see Fig. 1).

## 3. LOCALISED CORROSION

In the safety analysis of disposal of spent nuclear fuel it has been assumed that the penetration rate will be very low and that it will decrease with time. The possible penetration rates have been estimated based on the measurements performed to items that have been buried underground for long periods of time. From these items the pitting factor $P_f$ has been determined as the ratio of the maximum pit depth and the average general penetration depth, determined from weight loss ($P_f = P_{max}/P_{av}$). The pitting factor has been found to be at a maximum 25, but this has been considered as a very conservative value. The pitting factor has also been estimated for archaeological artefacts, e.g. copper coins, but in these cases the average penetration rate is impossible to define because the original dimensions of the items are not known, and so the pitting factor is only

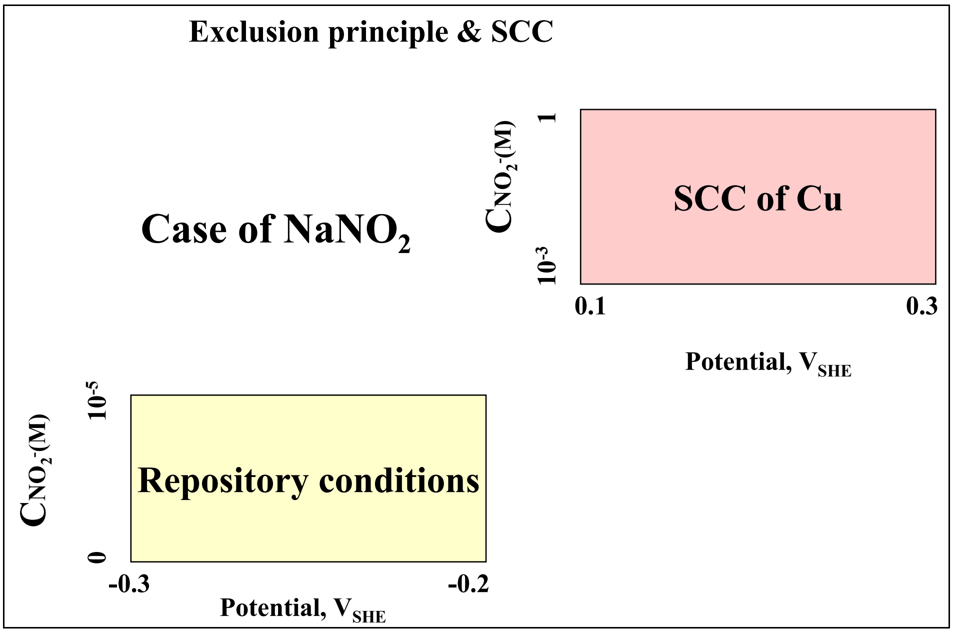

*Figure 1. Comparison of the experimentally determined range of potential and nitrite ion concentration causing suscebtibility to SCC in Cu and the estimated repository conditions.*

a guess. It is also good to remember that the concept of a pitting factor is not reasonable to use when pitting or general corrosion is only slight.

As pitting of copper has almost exclusively been reported to occur in the region where Cu(II) can be formed, i.e. under oxygenated conditions, also longer term exposure tests under oxygenated conditions would be needed to assess the propability of occurrence reliably. A possible mechanism for pitting of copper in low potential conditions containing sulphide ions has been recently proposed (Hermansson and Eriksson, 1999). It is however still unclear whether the mechanism is operable in repository conditions.

The studies reported in the literature for different environments (Ribotta et al., 1995, Sanchez-Perez et al., 1990) indicate that $HCO_3^-$ ions increase the solubility of copper in the stability region of Cu(II), possibly by complexing the divalent copper ions. Thus they can be concluded to render the oxide film formed on copper susceptible to local damage and to localised corrosion at positive potentials.

The concentration of bicarbonate ions in the borehole analysis in Finland has been found to be between 25 mg/l and 400 mg/l (Anttila et al., 1999a and 1999b). According to some recent experimental results (Sirkiä et al., 1999) the stability of the oxide film can be questioned at high potentials in the presence of 100 mg/l $HCO_3^-$ ions. Thus, the repository conditions may lie in the concentration window for susceptibility to localised corrosion. Another factor to be taken into account when considering the possibility to exclude the occurrence of localised corrosion is the potential. The potential where Cu(II) may start to form at the expected slightly alkaline pH of 7.5 to 8.5 is +0.07 to +0.14 $V_{SHE}$. These potentials are about 0.3 to 0.4 V higher than the measured natural redox potential for anoxic environment in the undisturbed condition of the bedrock. Thus, for this condition there seems to be no overlap of the potentials with the potential window for susceptibility to localised corrosion (see Fig. 2).

Higher positive potentials may however be relevant in repository conditions in case of the oxygen containing period immediately after the closure of the repository or during flushing of the repository with fresh oxygenated water e.g. during an ice age. Such a period with oxygenated conditions can be expected, depending on the source, to last from a couple of weeks to 30 years after which all the oxygen is consumed and anoxic conditions resume. Accordingly, a possible hazard caused by bicarbonate ions to the stability of copper oxide films cannot be totally excluded during such a period. Therefore, the next step in assessing the propability of occurrence of localised corrosion would be to check first if such high positive potentials are achievable in repository conditions, and second to verify with longer term experiments at the highest achievable potential if a real risk exists for pitting by bicarbonate ions in simulated oxygenated repository conditions.

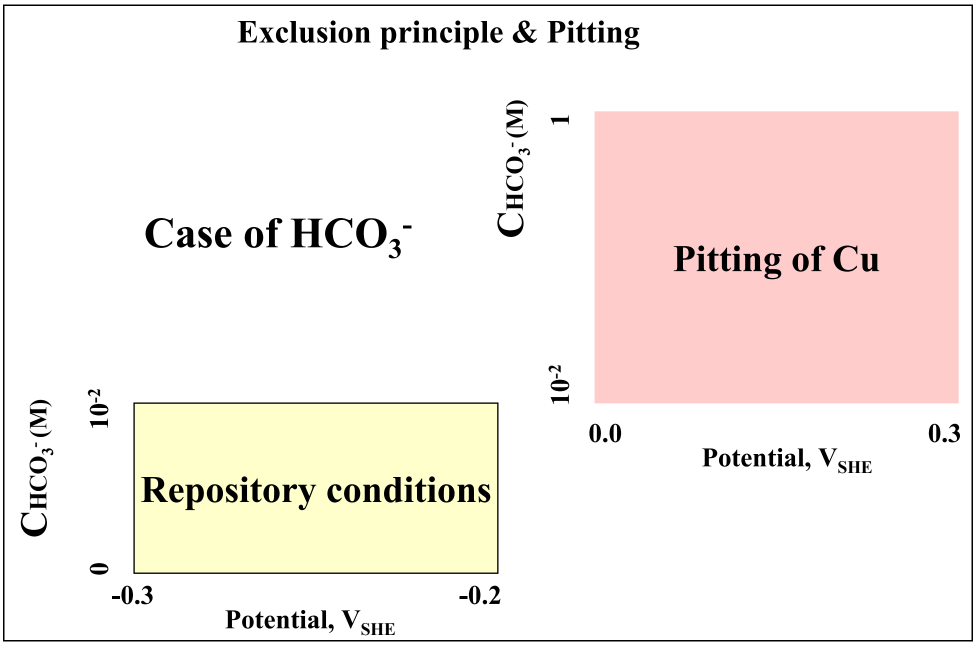

*Figure 2. Comparison of the experimentally determined range of potential and bicarbonate ion concentration causing suscebtibility to pitting in Cu and the estimated repository conditions.*

## 4. GENERAL CORROSION

The occurrence of general corrosion of copper cannot be excluded in repository conditions. It has for instance been recently predicted (Beverskog and Puigdomenech, 1998) on the basis of thermodynamic calculations that copper dissolves actively in highly saline environments even in anoxic conditions. However, thermodynamic calculations do not give any estimate for the actual corrosion rate. Accordingly, one has to arrive at either experimental or theoretical results showing that the rate of general corrosion is acceptably low to prove the suitability of copper as a shield material. Taking the corrosion allowance of the copper canister as 50 mm and the demanded life time of 100,000 years, the allowed maximum corrosion rate is $5*10^{-4}$ mm/year.

Recent experimental studies (Laitinen et al., 2001, Saario et al., 2001) in simulated repository conditions (80 °C, 14 MPa) have reached a conclusion that active dissolution of copper does take place both in highly saline (5.4 % $Cl^-$) and saline (1.4 % $Cl^-$) simulated ground water. The corrosion rate measured in weight loss coupon tests of relatively short duration (7 days) has been found to be $2*10^{-2}$ mm/year. This corrosion rate would indicate a lifetime of roughly 2500 years. This is clearly lower than the required 100,000+ years. However, such an estimate rests on the assumption that the transport rate of the reactants (e.g. oxygen containing species) towards the surface and that of reaction products (cuprous ion complexes) away from the surface are fast enough to allow the corrosion process to proceed. However, it is likely that the bentonite layer next to the copper surface will act as a diffusion/migration barrier slowing down the transport. To draw more definite conclusions, this needs to be experimentally verified and supported by theoretical modelling of transport in bentonite.

## 5. CONCLUSIONS

We describe in the present paper an approach for dealing with the three forms of corrosion that may pose a risk for the stability of the copper canister in the repository conditions, namely stress corrosion cracking, pitting corrosion and general corrosion. The approach is based in an attempt to find out whether the occurrence of any corrosion type can be excluded in the disposal conditions. If this is not the case, the next step is to evaluate whether the maximum extent of corrosion is below an acceptable limit. In case of potential risks, more detailed mechanistic and quantitative corrosion studies are recommended. This leads to a slightly different research strategy for each form of corrosion.

Stress corrosion cracking has been considered as a mechanism that cannot be allowed to occur, and therefore the exclusion principle has been chosen for this type of corrosion. The exclusion principle, involving concentration, potential and stress level as variables has successfully been applied to exclude the possibility of stress corrosion cracking caused by nitrite ions. In the case of other known species that may cause stress corrosion cracking in pure copper, i.e. ammonium ions and acetate ions, the situation is different, and more experimental data is needed in order to be able to exclude the risk caused by them.

Pitting corrosion of copper has been reported to occur almost exclusively at high positive potentials where Cu(II) can be formed and may dominate in the passive film on copper. These potentials are thought to be not achievable in the repository conditions. However, a solid experimental proof for this is not yet available. In addition, the recently proposed mechanism of localised corrosion of copper in anoxic conditions  in the presence of high amounts of sulphides needs to be further investigated. If this mechanism were proven to be valid, the next step would be to use the exclusion principle with regard to the concentration of the sulphide species causing the phenomena.

General corrosion has been indicated to take place at an unacceptably high rate in highly saline environments that are representative of some possible ground water environments. These findings call for an experimental and theoretical verification of the transport rate of oxygen to the reacting surface and of the corrosion product away from the surface under realistic repository conditions.

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# Canister Fabrication and Emplacement Issues Related to Isolation

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In the next several years, SKI will review SKB's license application for the proposed canister Encapsulation Facility for spent nuclear fuel, as well as a license application for an underground SFL-2 repository. These reviews will include evaluation of SKB's detailed analyses and demonstrated reliability of the processes and methods employed for:

- canister fabrication,
- canister closure by a yet-to-be-finalized welding method,
- non-destructive testing of weldments,
- emplacement of canisters with surrounding bentonite-based buffer, and
- performance assessment modeling of fabricated canisters as emplaced in the repository.

SKB must select reference materials and fixed dimensions for the canister, and demonstrate standardized methods for welding and weld testing, since these choices will greatly influence the design of the Encapsulation Facility. Furthermore, it is reasonable to expect that SKB will have conducted sufficient canister fabrication and post-fabrication analysis for a full-scale canister design to demonstrate that these reference techniques can be suitably scaled-up to a successful serial-production process within the Encapsulation Facility. In addition, it is anticipated that SKB will define acceptable specifications for manufacturing, closure, defect structure determination (flaw sizes, spatial distribution, frequency), and non-destructive testing (NDT), to be conveyed to SKI for review well in-advance of the Encapsulation Facility license application. Likewise, specifications and limited-demonstration regarding successful transport and emplacement of sealed waste canisters and surrounding buffer are foreseen for the repository license application, as well as quality assurance/ quality control (QA/QC) methods by which successful emplacement of undamaged barriers will be confirmed.

Both canister weldments and reliable emplacement of the EBS (canister + buffer) are issues of critical significance to the overall isolation performance of the planned SFL-2 repository. This is because of the expected long lifetime (~$10^6$ years) of the welded outer-copper shell of the canister, which in turn relies on the physical integrity of the low-permeability buffer that assures diffusive mass-transfer constraints on the long-term rate of copper corrosion. While SR'97 is based on long-term corrosion of the base metal (bulk copper walls), it is recognized that the weldments of the canister may have a statistical distribution of fabrication flaws leading the initial or early-time («10,000 years) failure of the canister. Thus, it is important for SKI to identify and examine fabrication, handling and testing issues for canisters, as well as methods for potentially resolving such issues, that can serve as the basis for a dialog with SKB leading up to the Encapsulation Facility and repository licensing applications.

Issues associated with fabrication, welding, testing and emplacement of waste canisters are common across international geological repository programs. The leading program in these areas is the US Yucca Mountain Project (YMP), which has a license application schedule over the next several years that is similar to that in Sweden. Despite obvious differences in materials and possibly welding methods, advanced US studies on evaluation of weldments, including flaw detection and characterization, provide a useful basis to identify potential issues and resolution strategies for the Swedish situation.

In addition, techniques on statistical analysis of welding fabrication flaws based on limited or episodic analysis have been developed and successfully applied in other industrial sectors (e.g., aircraft, nuclear reactors). In particular, the statistical basis for extrapolating non-destructive testing (NDT) measurements to bound the number, size, and location of flaws in reactor vessel materials has been extensively developed and refined by both nuclear power utilities and nuclear regulatory agencies. These studies have focused on ferritic materials different from copper, and welding methods possibly different than those that may be used by SKB. Nonetheless, the conceptual basis demonstrated in these studies for linking NDT to weldment flaws distributions, as well as the evolution of flaws under expected operating (repository) conditions, can provide a basis for initial perspective for SKI/ SKB technical discussions on this topic.

Finally, issues associated with vertical (or possibly horizontal) emplacement of canister and buffer are also of concern. Irregular or damaged emplacement of the buffer is especially problematical, and QA/QC methods or design modifications to assure avoidance of such problems are not yet established.

# ANALYZES OF COUPLED HEAT AND MOISTURE FLOW IN UNSATURATED AND SATURATED BENTONITE

**Claesson**[1]

Extended Abstract for SKI Workshop, Nov. 2002

## 1 Coupled heat and moisture flow

The bentonite layer, that surrounds and protects the canisters in a nuclear waste repository deep down in rock, experiences a complex coupled heat and moisture flow process. The released heat from the canister will cause an initial drying. The water 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. Further studies and deeper understanding of these processes have been called for by SKI.

A way to contribute to this aim is to develop more special analyzes, mathematical solutions ands models that address key issues from different points of view.

Large computer models involving many coupled processes require careful testing and validation. An example is the termo-hydro-mechanical processes in nuclear waste repositories in rock, and in particular the intricate water-temperature-pressure processes in the bentonite layer between canisters and rock. The transport coefficient for moisture flow may increase by orders of magnitude from dry to wet conditions. There is a need to test that the models give correct results when the property functions involved in the calculations vary strongly with the state variables.

The purpose of this study is to provide a such analyzes and particular solutions, which are quite accurate and obtained in a completely different way. The solutions give new tools of analysis, which provide further insight into the complicated coupled, highly non-linear processes with water evaporation and condensation. The effects and relative importance of particular assumptions and choice of data may be analyzed in a very direct and rapid way.

## 2 Tasks and goals

The *tasks and goals* of this study are the following:

- Water saturation of the bentonite. Development in space and time. Time-scale?
- Drying. Under what conditions? To what extent? What is required to prevent drying?
- Identify key parameters for the saturation and drying processes.
- Perform sensitivity analyzes.

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[1] Studies in cooperation with Carl-Eric Hagentoft, Building Physics, and Göran Sällfors, Geotechnical Engineering, Chalmers.

- Provide solutions with high and controlled accuracy to test other models.

We will here study the following cases:

- Initial drying at the warm canister side and water saturation from the rock side
- Generalized Boltzmann solutions
- Steady-state solution for coupled radial flows

## 3 Equations

The moisture flux $g(r,t)$ (kg $H_2O/m^2s$) in the bentonite has a liquid and a vapor component. The liquid flux $g_\ell$ is proportional to the pressure gradient with a hydraulic conductivity $k(S)$ that is a function of the degree of water saturation $S = S(r,t)$. The flux is inversely proportional to the temperature-dependent viscosity $\eta(T)$. The water vapor flux $g_v$ is proportional to the gradient of the water vapor density $\rho_v$ in the gas phases in the pores with a vapor conductivity factor $D_v(S)$ that is a decreasing function of $S$. We have:

$$g_\ell = -\frac{\rho_w k(S)}{\eta(T)} \cdot \frac{dP}{dS} \cdot \frac{\partial S}{\partial r}, \qquad g_v = -D_v(S) \cdot \frac{\partial}{\partial r}[\rho_v(P,T)], \qquad g = g_\ell + g_v. \tag{1}$$

The enthalpy flux $q$ ($J/m^2s$) has a conductive part with a thermal conductivity $\lambda_m(S)$ that is a function of $S$. The convective part is equal to the liquid and vapor fluxes multiplied by their respective heat contents. We have

$$q = -\lambda_m(S)\frac{\partial T}{\partial r} + h_\ell(T)g_\ell + h_v(T)g_v. \tag{2}$$

Using the water retension curve $P(S)$, the gas law and Kelvin's law relating water pressure to relative humidity, etc, the flow equations may be written:

$$g(r,t) = -K_S(S,T)\frac{\partial S}{\partial r} - K_T(S,T)\frac{\partial T}{\partial r}. \tag{3}$$

$$q(r,t) = -\lambda_S(S,T)\frac{\partial S}{\partial r} - \lambda_T(S,T)\frac{\partial T}{\partial r}. \tag{4}$$

The four functions for the flow coefficients, $K_S$, $K_T$, $\lambda_S$ and $\lambda_T$, become functions of $S$ and $T$. These functions depend on the particular assumptions and on the particular data for bentonite and water.

The conservation equations for the moisture content $\phi\rho_w S(r,t)$ and the enthalpy content $h(r,t)$ ($J/m^3$) are in the radial case

$$r\phi\rho_w \cdot \frac{\partial S}{\partial t} = -\frac{\partial(rg)}{\partial r}, \qquad r \cdot \frac{\partial h}{\partial t} = -\frac{\partial(rq)}{\partial r}. \tag{5}$$

The considered process[2] is a complicated one with coupled, highly nonlinear flows that involve many things. There are liquid flow and vapor flow as well as conductive and convective heat flow depending on gradients in pressure, water vapor density and temperature, (1)-(2). The flow coefficients depend on water properties such as saturation water vapor pressure $p_{\mathrm{sat}}(T)$, heat of

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[2] This study uses the data and basic models from Rutqvist et.al. Coupled Thermohydromechanical Analysis of a Heater Test in Saturated Clay and Fractured Rock at Kamaishi Mine, SKI Report 99:50, and Jing et.al. DECOVALEX II PROJECT, Technical Report - Task 2C, SKI Report 99:23.

evaporation $L_{\mathrm{ev}}(T)$, heat or enthalpy content $h_\ell(T)$ and $h_v(T)$ for liquid water and water vapor, and dynamic viscosity of water $\eta(T)$. They also depend on the properties of bentonite: water retention curve $P(S)$, hydraulic conductivity $k(S)$, water vapor diffusion coefficient $D_v(S)$, and thermal conductivity $\lambda_m(S)$. Here, $S$ is the degree of water saturation. With Kelvin's relation, the water vapor density in the gas phases of the bentonite pores becomes a function of $P$ and $T$: $\rho_v(P,T)$. The total enthalpy becomes a function of $S$ and $T$.

All these functions of $S$ and $T$ are in the models represented by explicit formulas, with a relative error compared to measured data that is shown to be below 1%. The formulas for the material properties of bentonite are easily changed to allow for other assumptions and tests of sensitivity.

## 4 Transient drying and saturation

We have made preliminary studies of the transient drying and saturation of the bentonite annulus, when it is exposed to heating from the canister side and water saturation from the rock side. These ongoing studies indicate that it may be possible to obtain an analytical solution for $S(r,t)$ and $T(r,t)$ with a relative error around or below 5-10%.

## 5 Generalized Boltzmann solutions

An exact time-dependent solution to the coupled nonlinear equations many be found in the plane case. We consider a semi-infinite bentonite layer with constant initial $S$ and $T$. At $x=0$ we impose a step change for $S$ and $T$. This is an important special case since all transient cases may be considered as composed of step changes. We have the conditions

$$\begin{aligned} &S(x,0)=S_{\mathrm{in}} \qquad T(x,0)=T_{\mathrm{in}} \qquad 0<x<\infty \\ &S(0,t)=S_0 \qquad T(0,t)=T_0 \qquad t>0 \end{aligned} \tag{6}$$

We consider solutions that are a function of $x/\sqrt{4t}$ only:

$$s=\frac{x}{\sqrt{4t}}: \qquad S(x,t)=\tilde{S}(s) \quad T(x,t)=\tilde{T}(s), \quad 0<s<\infty. \tag{7}$$

The time factor cancels and we get after some calculations the following set of equations

$$\begin{aligned} &\phi\rho_w\cdot 2s\cdot\frac{d\tilde{S}}{ds}=\frac{d\tilde{g}}{ds} \qquad\qquad 2s\cdot\frac{d}{ds}[h(\tilde{S},\tilde{T})]=\frac{d\tilde{q}}{ds} \\ &\tilde{g}(s)=-K_S(\tilde{S},\tilde{T})\cdot\frac{d\tilde{S}}{ds}-K_T(\tilde{S},\tilde{T})\cdot\frac{d\tilde{T}}{ds} \\ &\tilde{q}(s)=-\lambda_S(\tilde{S},\tilde{T})\cdot\frac{d\tilde{S}}{ds}-\lambda_T(\tilde{S},\tilde{T})\cdot\frac{d\tilde{T}}{ds} \end{aligned} \tag{8}$$

We get four *ordinary*, coupled, non-linear, first-order differential equations for $\tilde{S}$, $\tilde{T}$, $\tilde{g}$ and $\tilde{q}$ as functions of $s$. We have four boundary conditions:

$$\tilde{S}(0)=S_0 \quad \tilde{S}(\infty)=S_{in} \quad \tilde{T}(0)=T_0 \quad \tilde{T}(\infty)=T_{\mathrm{in}} \tag{9}$$

This set of equations may be solved in any mathematical program. We have implemented the solution in Mathcad. An accuracy of the order 0.1 % may be obtained. We have an independent solution to test other numerical codes. The solution is also quite useful for analyzes. We have obtained another handy tool for analyzes of heat and moisture processes in the bentonite layer.

# 6 Steady-state solution for coupled radial flows

We consider the annular region of bentonite from canister to rock. The time scale to attain a steady-state temperature profile, if constant temperatures were to be imposed at the boundaries of the bentonite layer with a thickness of 0.35 m, is some 7 hours. This means that we may, with very high accuracy, consider the thermal process as a quasi steady-state one with a constant $Q_c$, which assumes different values depending the considered time from deposition. The moisture flow process, if *constant* conditions were to be kept at the boundaries of the bentonite, has a time scale of a few years to approach a steady-state moisture profile. This means that the whole process is a quasi steady-state one after a few years from deposition, as the moisture state in the neighboring rock mass changes slowly,except during an initial phase.

An important model is obtained by considering *steady-state* solutions in the annular region from canister to rock. The modeling is then simplified considerably. But many of the basic complications and features remain. Initial transient processes during the first few years will have steady-state solutions as limits towards which they tend. We get a good deal of information about the transient part, and in particular about the largest drying that may occur.

## 6.1 Coupled ordinary differential equations

The total radial fluxes $G = 2\pi rH \cdot g$ and $Q_c = 2\pi rH \cdot q$ are in the considered steady-state processes *constant*, i.e. independent of the radius $r$. The canister is impermeable to moisture flow, which means the $G$ is zero. We have for all $r$ in the annular bentonite region from the canister radius $r_\mathrm{c}$ to the radius at the rock boundary $r_\mathrm{r}$:

$$g = 0 \quad (\text{ i.e. } g_\ell(r) = -g_v(r)\ ), \qquad q(r) = \frac{Q_c}{2\pi rH}, \qquad r_\mathrm{c} \le r \le r_\mathrm{r}. \tag{10}$$

We have to solve the equations (3-4) for the fluxes (10). The equations for $S(r)$ and $T(r)$ become

$$K_S(S,T)\frac{dS}{dr} + K_T(S,T)\frac{dT}{dr} = 0, \tag{11}$$

$$\lambda_S(S,T)\frac{dS}{dr} + \lambda_T(S,T)\frac{dT}{dr} = -\frac{Q_c}{2\pi rH}. \tag{12}$$

We have got two *coupled ordinary* differential equations for the degree of saturation and the temperature as a function of the radius $r$. The values of $S$ and $T$ at $r = r_\mathrm{r}$ are specified:

$$S(0) = S_\mathrm{r}, \qquad T(0) = T_\mathrm{r}. \tag{13}$$

The two coupled, highly nonlinear, first-order ordinary differential equations are solved using the mathematical program Mathcad. The Mathcad model is a handy and quite versatile tool of analysis. The model and its application has been reported in a draft report.

A reference case is studied in detail. The relative errors of the whole solution are shown to be of the order $10^{-4}$ or smaller. We have a model with very high and controlled accuracy that may be used to test other models.

A systematic variation of the parameters that influence the process is presented. Important parameters for the drying are the prescribed degree of saturation and temperature at the rock boundary, and the heat release from the canister. A critical and quite sensitive factor is level of the ratio between the vapor and liquid flow conductivity coefficients ($D_v(0)/k(1)$). *All* other factors were found to be of moderate or negligible importance (in the present model). For $S_r = 1$ we get $S = 1$ throughout the bentonite (in steady-state). Rather strong drying occurs in some of the studied cases for $S_\mathrm{r} < 0.95$. The model provides a lot of information about the conditions when drying occurs and when it is negligible.

## 6.2 Coordinate-independent relation between $S$ and $T$

Equation (11) involving $S(r)$ and $T(r)$ is actually a relation between $S$ and $T$, since the differential $dr$ cancels.We have in the temperature interval from the rock temperature $T_{\mathrm{r}}$ to the higher temperature $T_{\mathrm{c}}$ at the canister

$$\frac{dS}{dT} = -\frac{K_T(S,T)}{K_S(S,T)}, \qquad T_{\mathrm{r}} \leq T \leq T_{\mathrm{c}}. \tag{14}$$

The relation between $S$ and $T$ becomes *independent* of the $r$-coordinate. The relations between degree of saturation as a function of temperature, $S = S(T)$, may be represented by a set of curves independently of the radial coordinate. A single chart covers *all cases* of prescribed $S_{\mathrm{r}}$ and $T_{\mathrm{r}}$, and all rates of heat release, for a wide temperature span for any particular set of the other data. The chart for the reference case and the temperature interval $20 \leq T \leq 100$°C is shown in Figure 1.

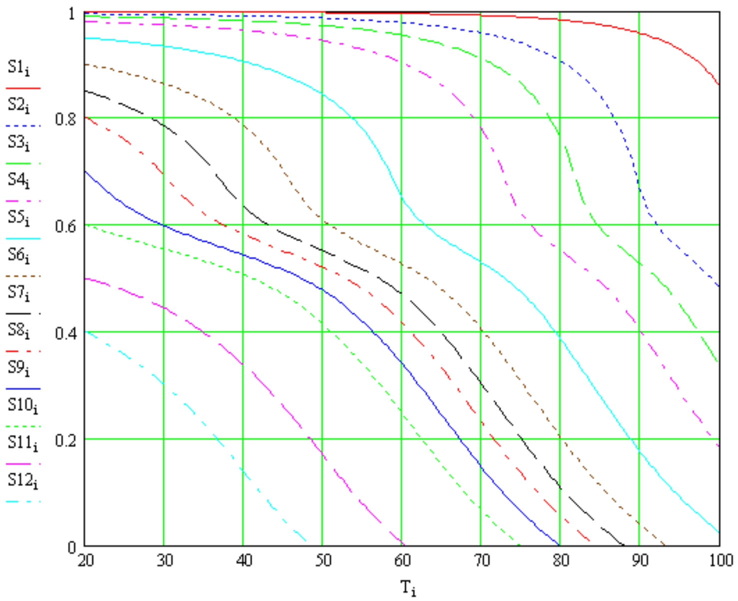

Fig. 1. Set of curves $S(T)$ representing all steady-state cases in $20 \leq T \leq 100$°C for the reference case.

STUDSVIK NUCLEAR AB
Korrosion Project
Hans-Peter Hermansson

Abstract
2002-10-29

## Corrosion experiments on copper in different groundwaters

A series of projects on copper corrosion has been performed at Studsvik on commission by SKI [1-4]. The work has been focused on general and localised corrosion of copper in the repository environment.

The work comprised a thorough compilation and up-date of literature data. A selection of a “working environment”, defining the chemical parameters and their ranges of variation was made from literature and discussions with SKI and later on used as a fundament for planning of experiments. Especially the importance of highly saline solutions and solutions containing sulphide was tested by thermodynamical calculations and laboratory experiments. Some of the results are highlighted here.

At simultaneous presence of sulphide and chloride a very complicated surface film is formed on the copper surface. In some cases of environment also the growth of copper containing whiskers was observed on top of the surface film. As whiskers could indicate an underlying localized attack on the copper metal, specific care was taken to find evidence of such attacks. The nature of layers and whiskers was investigated by applying SEM-EDS, XRD and Raman Spectroscopy. An example of layer and whisker morphology is shown in Figure 1.

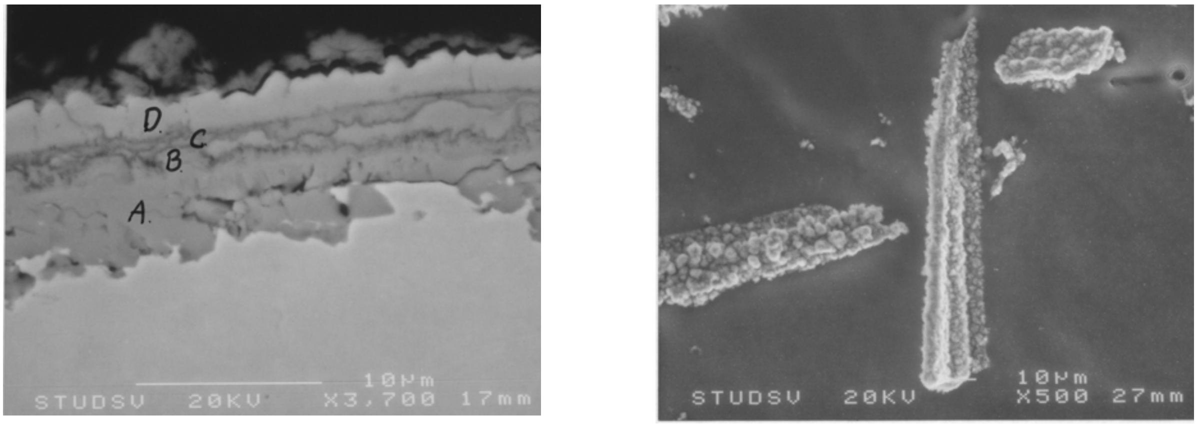

**Figure 1** Morphology of layer and whisker growth on copper. A-D in the left picture denote different strata in the layer. Parts of whiskers are shown in the right picture.

The two outer strata C and D contain sulphur. The next inner stratum B seems to contain a smaller amount of sulphur than the outermost. Those outer layers probably consist of copper sulphides, e.g. $Cu_2S$ in the B sub-stratum and CuS in the C and D sub-strata. However, many Cu-S containing phases are possible as well as more complicated phases. Stratum A, under the sulphur rich layers, probably consists of copper oxide, as sulphur is not present closest to the metal. The concentration of sulphur thus seems to increase outwards in the layer structure. The B stratum is easily scaled off from stratum A, which could confirm a change from oxide to sulphide types of phases in the strata.

Another part of the work was done to further develop knowledge about the thermodynamic limits for copper corrosion in the repository environment. A rough overview of the chemical system Cu-Fe-Cl-S-C-H-O was therefore made. The study indicated that a good passivating film is formed on copper only at a low chloride concentration in a sulphide free environment. High chloride concentrations can prevent formation of a passive film and also destabilise a passivating oxide film that is present from the beginning. Copper sulphides can be formed at low potentials causing passivating films that are poor. The only protection against dangerous general corrosion at high chloride and sulphide concentrations would therefore be shortage of oxidising agents and low transportation rates of reacting species.

The film formation and whisker growth were studied more in detail. The oxide type of film formation on the copper surface in groundwater is a slow process taking weeks or months. The chloride concentration affects the rate of formation and the morphology of the film formed. In the presence of sulphide the surface processes are much faster and sulphide type of film formation takes only minutes to hours.

In the high chloride/sulphide solutions a multitude of easily detached and very fragile whiskers or needle-shaped growth forms was often found on the surface. An example of those is shown in the right hand side of Figure 1. A whisker seems to have a core of copper sulphide. The concentration of sulphide increases from the root to the top part of the whisker. There are often straight dendritic, flanged edges along the sides of the whiskers. In the case shown in Figure 1 they are rich in copper oxide and carbonate. The composition of a whisker is thus very complex. A similar stratification as found in the corrosion layer is also present in a whisker but with a concentric, cylindrical geometry.

When analyzing the corrosion layer, all the fragile whiskers fell off. Because of this no obvious roots or substrate areas for whisker growth could be found. It could be speculated if each of the numerous pits observed beneath the layers is situated below a whisker and is part of a whisker substrate or root, but this speculation has not yet been confirmed. Future experiments will be performed to test the speculation.

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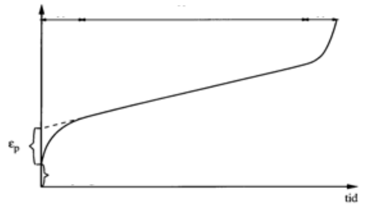
# Models for creep and creep fracture in copper.

An extended abstract of a presentation at the SKI workshop on the Long Term Integrity of the KBS-3 Engineered Barrier System, Nov. 6-8, 2002.

Kjell Pettersson, Matsafe AB

*Models for creep.*

Creep is usually defined as the time-dependent plastic deformation of a material. Experimentally a creep test is performed by measuring the time dependent elongation of a tension specimen at a constant stress, which in the practical application normally means constant load. The typical result of a creep test is seen in the attached figure. After a rapid initial deformation the material deforms at a constant rate for some time until the rate increases again until fracture occurs. The constant creep rate, the secondary creep rate, is normally described by Norton's law:



$$\varepsilon = AD\left(\frac{\sigma}{\sigma_0}\right)^n = AD_0 \exp\left(-\frac{Q}{RT}\right)\left(\frac{\sigma}{\sigma_0}\right)^n \qquad (1)$$

It is usually a form of Norton's law which is used in calculations of creep deformation. However creep in the copper canister for nuclear waste takes place at low temperature where the parameters in the Norton equation are determined at relatively high strains, strains which are higher than those expected to occur in the canister. It is therefore proposed that creep or plastic deformation should be modelled from the principle that the strain rate is the result of the applied stress and the microstructural state of the material. This principle is illustrated by the present model where the dislocation density is taken as a characteristic parameter for the microstructural state. Thus the strain rate is determined by

$$\varepsilon = \varepsilon_0 \exp - \frac{H(\sigma^*)}{kT} \quad \text{where} \qquad (2)$$

$$H(\sigma^*) = H_o - \frac{b^2 \rho^{-1/2}}{\overline{m}}\left(\sigma - \sigma_o - \alpha_m G b \sqrt{\rho}\right) \qquad (3)$$

The dislocation density develops with strain and time according to

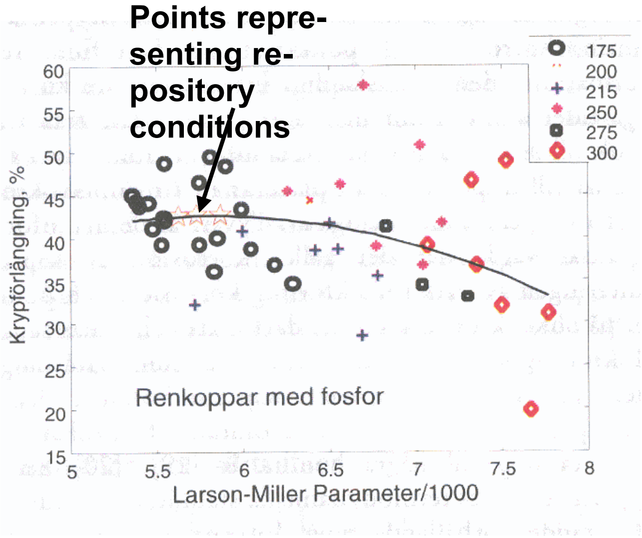
$$\frac{d\rho}{dt} = \varepsilon \cdot \frac{d\rho}{d\varepsilon} - MD_s\rho^2 \tag{4}$$

$$\frac{d\rho}{d\varepsilon} = \frac{\overline{m}}{bs} - \Omega\rho - A\rho^2 \tag{5}$$

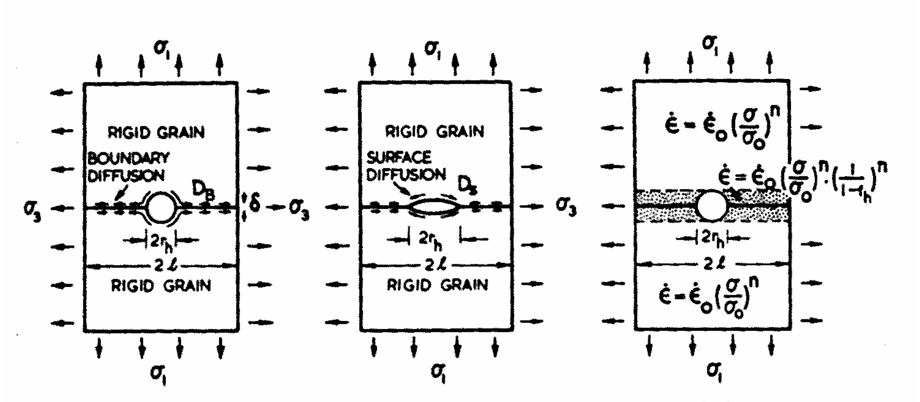
This is a set of differential equations which can be applied to arbitrary applied loading or deformation sequences. Specifically the equations were applied to experimentally determined stress-strain curves and creep curves in order to determine values of unknown parameters. This set of parameters was subsequently used to rather successfully reproduce experimental creep curves determined at other stresses and temperatures (Pettersson 1995).

*Modelling of creep fracture.*

Quite frequently a creep test is terminated by fracture at a very low strain. In such cases the fracture path goes in the grain boundaries of the material. The cause of fracture is the nucleation and growth of small cavities in the boundaries. Early creep tests of oxygen free copper intended for the waste canister resulted in creep failures at strains between 0.2 and 0.9 %. Subsequently it was discovered that if 30-50 ppm of phosphorus was added to the material the creep rate was reduced and the mode of failure was a normal ductile failure. There is still however a need for predicting the behaviour of the improved copper under long times under load. The figure below (Sandström 2001) is a prediction of the failure strain of copper with a P addition under repository conditions. It indicates that the failure strains will be of the order of 40 % under repository conditions. Thus there seems that there is no risk for creep failure of the copper canister. However it may be noted that this extrapolation is based on creep test series of copper in which no low ductile failure has occurred. One may ask whether this low ductile failure mode is intimately coupled to the ductile failure mode or if it is a process which operates in parallel with the ductile mode. If the latter is the case there is actually no firm basis for concluding that the low ductile failure will not occur in the copper canister. In order to illustrate how data on low ductile failure might be used for extrapolation,the following analysis has been carried out based on the creep results for copper without the phosphorus addition (Henderson 1991).



The analysis is based on a review on creep fracture by void growth (Cocks 1982). Cocks and Ashby identifies three modes of void growth according to the figure below:



(a) **Bounday diffusion** (b) **Surface diffusion** (c) **Power-law creep**

If the theories for the three modes of failure are applied to the copper creep data the time to failure is overpredicted by several orders of magnitude for the two diffusion controlled modes. For the power law creep mode the overprediction is of the order 50 for material with 10 ppm S while the theory seem to hold for material with 6 ppm S. However the prediction of life at 50 MPa and 100 °C is still only about 25000 years which causes some concern. It would be interesting if some low ductile creep data for the P added copper was obtained so that the life for that particular failure mechanism could be extrapolated to repository conditions.

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# DECOVALEX Simulations Results Related to EBS

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## Introduction

Over the past decade SKI supported a collaborative research effort between Lawrence Berkeley National Laboratory (LBNL) and the Royal Institute of Technology (KTH) to provide SKI with independent codes and model experience for investigation of SKB's work on EBS. The emphasis is on coupled thermo-hydro-mechanical (THM) processes in the bentonite buffer and surrounding rock mass.

Two numerical models are adapted and utilized for the studies of EBS. The first one is ROCMAS, which is a finite element code for three-dimensional analysis of coupled THM processes of unsaturated/saturation porous and fractured geological media (Rutqvist et el. 2001). A version of this code has been tailor-made for a rigorous analysis of EBS including bentonite swelling and rock interaction. The second code is TOUGH-FLAC, which has the capability of solving coupled THM problems under multi-phase flow conditions. The multi-phase flow capability means that it can used for studying migration of gas and its interaction with the liquid in more detail (Rutqvist et al. 2002). The TOUGH-FLAC code utilizing two established codes; TOUGH2 for TH analysis and FLAC3D code for rock and soil mechanics analysis. Both ROCMAS and TOUGH-FLAC are currently applied to various problems within the DECOVALEX project.

The ROCMAS code has been extensively applied within the DECOVALEX I, II and III projects. In DECOVALEX I, the ROCMAS code was applied to solve two test cases on coupled HM behavior of single fractures (TC2 and TC6). Also in DECOVALEX I, the ROCMAS code was applied to simulate BMT2, which was a bench mark test on coupled THM behavior in a fractured porous medium. However, DECOVALEX II and III have been most developmental regarding the EBS because it involves major field experiments that focuses on the EBS and near-field rock mass behavior. These field experiments are:

1) The Kamaishi Mine heater test in Japan
2) The FEBEX experiment at the Grimel Test Site in Switzerland
3) The Drift Scale Heater Test at Yucca Mountain in Nevada

These experiments have been, or are currently analyzed using either ROCMAS or TOUGH-FLAC. Some of the results and findings are presented below.

### The Kamaishi Mine heater test

In DECOVALEX II, the ROCMAS code was applied for simulation of the Kamaishi Mine heater, which was a major THM experiment focusing on the EBS. The Kamaishi Mine heater experiment was conducted in a 10 meters long, 5 meters wide and 7 meters high alcove, excavated from an existing drift located at a depth of about 250 meters in a granitic rock mass. In 1995, a vertical test pit, 1.7 meters in diameter and 5 meters in depth, was drilled in the floor of the alcove (Figure 1a). The following year, an electric heater was installed into the test pit and surrounded by a buffer of bentonite clay. The bentonite was placed in layers of 0.1 meters with compaction of each layer to a dry density of about 1600 kg/m$^3$, which conditions the buffer to an initial gravimetric water content of about 15%. After the entire test pit was filled, a watertight concrete lid was placed on the drift floor, which in turn was supported by steel bars from the ceiling of the drift (Figure 1a). At the end of 1996, a flooding pool was set up on the drift floor and the heater was turned on with the temperature set to 100$^{o}$C. During a heating period of 8.5 months followed by a 6-month cooling period, system responses–including temperature, moisture content, fluid pressure, stress, strain and displacement–were monitored with several hundred sensors in both the buffer and surrounding rock mass. The experiment was completed in the beginning of 1998.

The Kamaishi Mine heater test motivated major development and adaptation of ROCMAS for modeling of coupled THM processes in unsaturated bentonite (Noorishad and Tsang, 1996). This included modeling of the important processes of vapor diffusion with evaporation and condensation in the bentonite coupled with moisture swelling and development of swelling pressure. The coupled analysis of the Kamaishi mine heater test involved coupled HM modeling of the excavation phase, coupled THM modeling of laboratory experiments on bentonite, and a full scale THM modeling of the heater test. The modeling of the excavation phase was also utilized for a model calibration of the *in situ* permeability of fractures intersecting the vertical test pit (Figure 1b). The laboratory tests of the benonite were used to test the capabilities of ROMCAS for modeling of coupled THM effects in bentonite, and also to back-calculate important bentonite properties to be used in the simulation of the full-scale heater test. Hence, the simulation of the full-scale heater test was conduced in three steps:

1) Calibration of *in situ* rock mass permeability again inflow measurements
2) Determination of bentonite properties in laboratory experiments
3) Blind prediction of the THM behavior of the bentointe buffer and rock mass during heating

The overall DECOVALEX II results of the modeling of the Kamaishi Mine heater test is summarized by Rutqvist et al. (2002b). In general, the modeling of the Kamaishi Mine heater test indicate that numerical modeling can provide highly confident results of temperature distribution, and reasonable highly confident results of the moisture flow in the bentonite and pressure distribution in the rock. The level of confidence decreases when interaction between multiple media (rock and buffer) are concerned and for prediction of the mechanical behavior of fractured rock in a low stress environment for near-field problems, as well as for the hydromechanical behavior of bentonite at low saturation. The result of all modeling

## The FEBEX experiment

Stephansson (2002) describes the setup of the FEBEX experiment in an accompanying extended abstract. This test is similar to the Kamaishi Mine heater test but it is larger in size and examines the concept of horizontal deposition holes. Furthermore, the bentonite buffer at FEBEX consist of prefabricated bentonite block, whereas bentonite powder was used at Kamaishi. The DECOVALEX II task of the FEBEX experiment is ongoing and so far the two of three subtasks have been completed. The first subtask involved prediction of transient coupled HM fluid pressure responses in the vicinity of the drift during its excavation, and thereafter inflow rate into the open drift. The second subtask involved modeling of the THM responses in the bentonite buffer during the heater test. Similarly to the simulation of Kamaishi Mine heater test, the analysis was conducted in three steps involving calibration of rock permeability again inflow measurements, determination of bentonite properties from laboratory tests, and a blind prediction of the THM responses during the heater test. The results of the blind prediction are similar to those at Kamaishi. The temperature can be predicted with high confidence, the moisture content can be predicted reasonable well, whereas the mechanical behavior of the buffer is the most challenging process to predict. The evolution of the stress in the buffer at FEBEX was slightly underestimated because of the influence of gaps between bentonite blocks.

The FEBEX experiment motivated further development of the ROCMAS code to include a so-called state surface model for a more accurate simulation of the mechanical behavior of the bentonite. A state surface model does not use a conventional single effective stress law but instead the volumetric expansion of the bentonite, which depends on two independent stress variables: the net stress (*in situ* stress minus gas pressure) and suction. The state surface model was tested against detailed laboratory experiments provided in the DECOVALEX II task definition.

## The Yucca Mountain Drift Scale Test

The setup of this experiment and the accompanying DECOVALEX II tasks are also described in the accompanying abstract by Stephansson (2003). The experiment is the largest of the three with a heater power about 40 times the one at FEBEX and the maximum temperature reaches about 200 °C at the wall of the test drift. The experiment is conducted in unsaturated rocks and has no bentonite buffer, which implies that the experiment in focused on THMC effects in the near field rock mass. From a coupled THM view point, one of the most interesting features of the Drift Scale Test is that changes in rock mass permeability is measured in regular intervals (about every three months) during the course of the heating. These permeability changes can be simulated using the TOUGH-FLAC code. It involves simulation of strongly thermally driven moisture movements with both wetting and drying of the fractured rock mass around the heated drift. A wetting of the fractures causes the air-permeability to decreases while drying causes the air-permeability to increase. At the same time thermal expansion of the rock mass creates thermal stress that tends to close fractures to smaller aperture. Thus, a prediction of the air-permeability changes during the heater test must consider both moisture content changes and mechanical closure or opening of fractures.

## Concluding remarks

In conclusion one may note that participation in the DECOVALEX project has been extremely valuable for developing and strengthening Ski's ability of an independent examination of SKB's works on EBS. Thus, SKi currently has available these two numerical models that have the same capabilities as SKB's numerical models, and in certain aspects far exceeds the capabilities of SKB's numerical models. This is important because SKI needs not only to investigate what SKB do but also investigate what they are not doing, thus providing them with insightful comments and guidelines.

Maybe the most important gain of the DECOVALEX project is the experience in solving realistic problems related to EBS, which provides experience and depths of knowledge for the future analysis of a real site. This is extremely valuable because the most important asset is not the numerical model itself (provided that it meats minimum requirements), but the knowledge how to adapt and apply the numerical model correctly for the specific problem.

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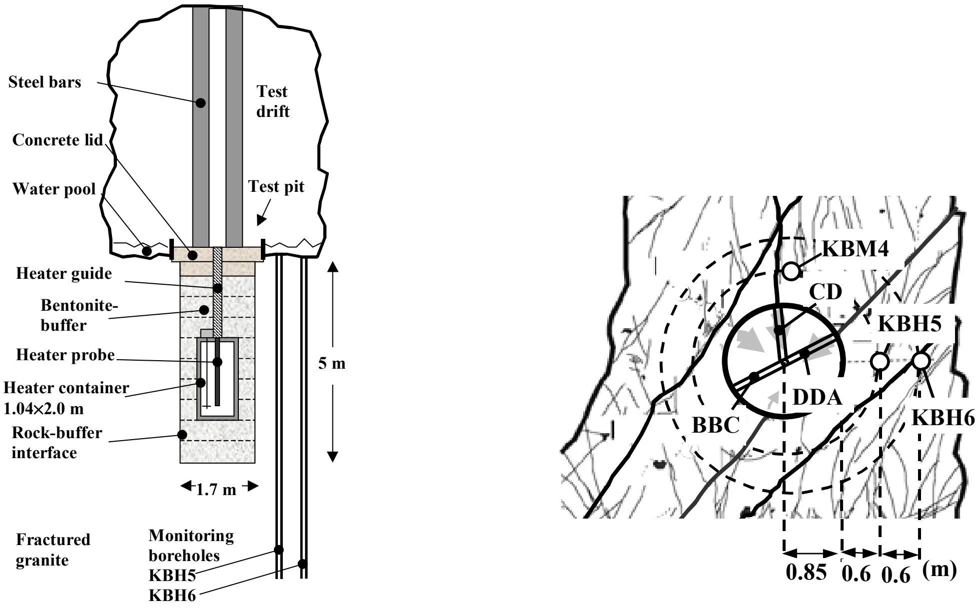
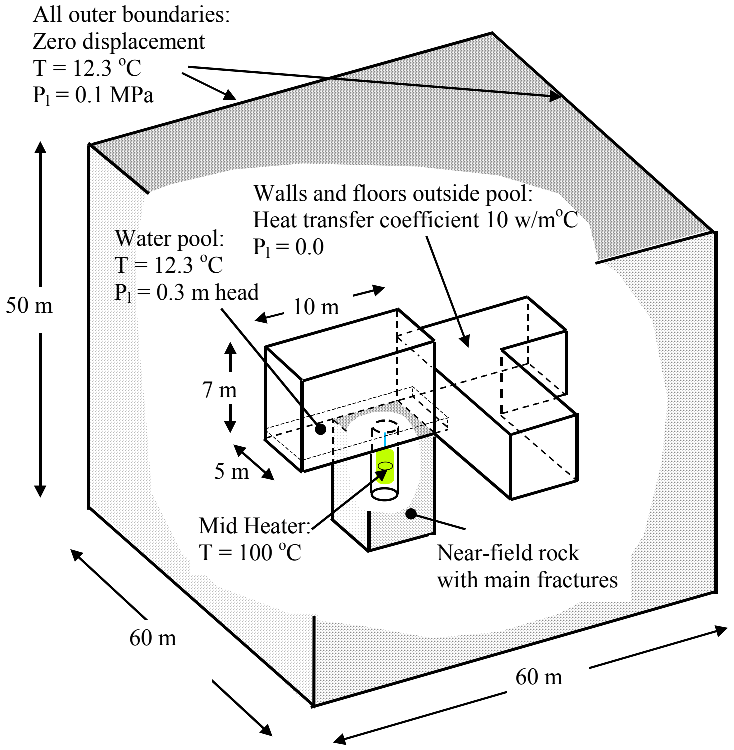


(a) Vertical section through the test pit

(b) Plane view of the floor of the test drift



c) Model of the Kamaishi Mine for simulation of the heater test with the ROCMAS code.

Figure 1. The Kamaishi Mine heater test.

# The Potential Impact of the Presence of Concrete upon the Performance of the KBS-3 Design

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Concrete will be used in the Swedish deep repository for spent fuel as a construction material, principally as plugs isolating sections of the disposal tunnels, but also as shotcrete, in rock bolts, and in grouts. SKB currently estimate that as much as 27 000 tonnes of concrete may be used in the repository, with the largest proportion (> 75 %, depending upon the final design) being used as concrete plugs (SKB, 1999). Although this amount of concrete is significantly less than that envisaged for SFL 3-5, it is worth considering the potential impact of this material on repository behaviour.

In addition to its properties as a low permeability barrier and its structural strength, concrete is a chemically-reactive barrier which may be deleterious to the long-term performance of other man-made or natural barriers in the deep repository. Its chemical reactivity derives from the hyperalkaline nature of entrained pore fluids due to the interaction of (principally) portlandite [$Ca(OH)_2$] and calcium silicate hydrate gel with ambient groundwater. Laboratory experimental and thermodynamic modelling evidence has shown that pore fluids in cement (concrete) may evolve from pH 13-13.5 buffered by the dissolution of trace sodium and potassium hydroxides, to pH 12.5 during removal of portlandite, and thereafter between pH 12.5 and pH 10 by removal of calcium silicate hydrate (C-S-H) gel. A typical pore fluid composition relationship with pore volumes of solvent for cement is shown in Figure 1. Depending upon the flux of groundwater and the mass of concrete, hyperalkaline pore fluids may persist for time periods in excess of $10^5$ years.

The persistence of elevated pH in pore fluids in concrete leads to the potential for reaction with the other engineered barriers in the repository and the host rock. Minerals in the buffer (montmorillonite, quartz, calcite *inter alia*) and the host rock (quartz, feldspars, sheet silicates, carbonates) have enhanced rates of dissolution and greater solubility at pH > 9, due to changes in aqueous and surface speciation of elements such as Si, Al, and C (e.g. Figure 2). Ion exchange and dissolution-precipitation processes accompanying migration of hyperalkaline pore fluids may lead to changes in physicochemical properties such as porosity, permeability and sorption behaviour. For example, model calculations have shown that cement pore fluids may advance ~60 cm through compacted bentonite before self-healing of porosity through growth of minerals such as calcium silicate hydrates, zeolites and sheet silicates over relatively short time periods (Figure 3).

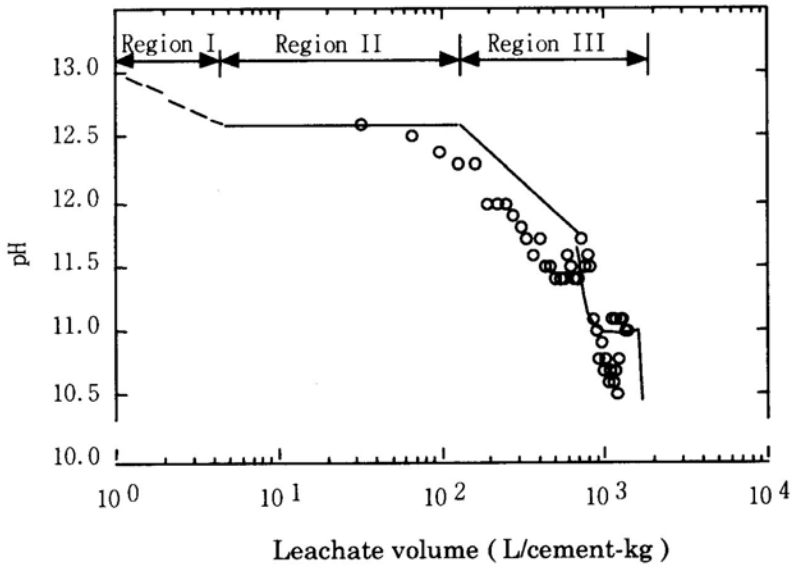

*Figure 1 Modelled (line) and experimental (circles) evolution of pH in cement with volumes of fluid leached. Region I corresponds to pore fluids dominated by dissolution of Na/K hydroxides; Region II to that buffered by portlandite dissolution; and Region III to that dominated by dissolution of C-S-H gel. From JNC (2000).*

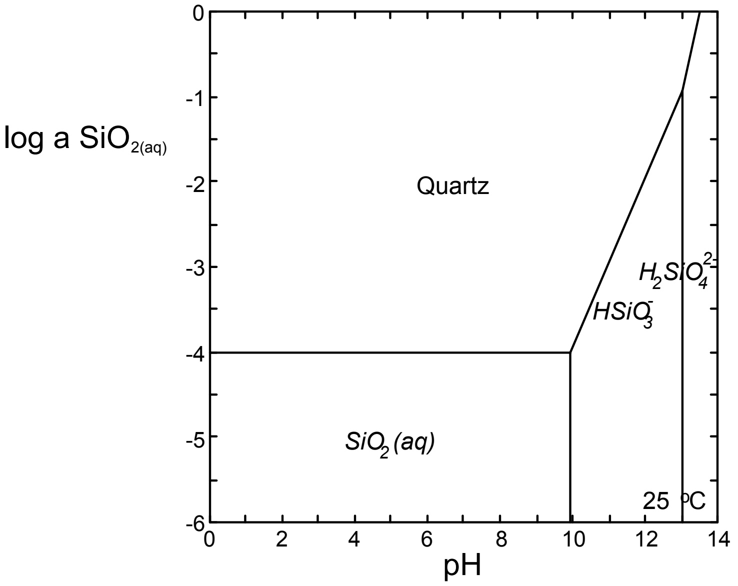

*Figure 2 Solubility of quartz and variation of Si speciation with pH at 25 °C. Note the steep increase in quartz solubility at pH > 10. The calculation was carried out using Geochemist's Workbench (Bethke, 1996).*

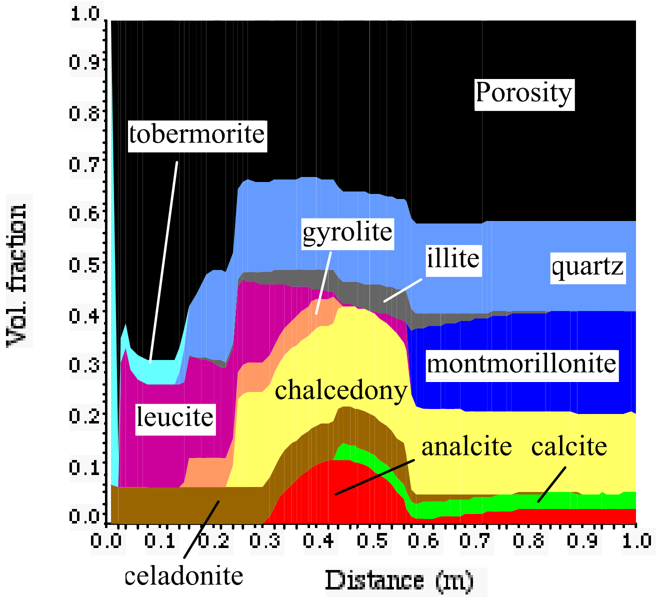

*Figure 3 Volume fractions of porosity and minerals versus distance for the simulation of cement pore fluid diffusion (left to right) and reaction with bentonite at 25 °C after 1000 years. The starting composition of bentonite is as per the right hand-side of the Figure. Leucite and analcite are zeolite-like minerals; tobermorite and gyrolite are calcium silicate hydrate minerals; chalcedony is a cryptocrystalline form of silica; illite and celadonite are non-swelling sheet silicates. From Savage et al. (2002). The calculation suggests significant perturbation of buffer mineralogy and porosity up to 60 cms from the contact with cement over a relatively short timescale.*

Consequently, mechanisms of pH buffering, and the interaction of hyperalkaline pore fluids with silicates are the subject of much on-going research. In particular, dissolution-precipitation kinetics and surface complexation reactions of silicate minerals, together with aqueous speciation of aluminium and silicon at elevated pH are all germane to the prediction of long-term performance through numerical modelling and the interpretation of relevant 'natural analogue' data (e.g. Smellie, 1998).

The behaviour of copper at high pH has received relatively little attention in the radioactive waste literature. In view of the location of the concrete plugs in the design for the deep repository, it is likely that any migrating cement pore fluids would be neutralised through reaction with the backfill and/or buffer mineralogy, prior to the copper canister being contacted. However, preliminary modelling indicates that copper predominates in Eh-pH space at pH 12, at Eh values less than –300 mV (Figure 4), suggesting that hyperalkaline pore fluids would not have a large impact upon copper stability unless accompanied by relatively oxidising redox conditions.

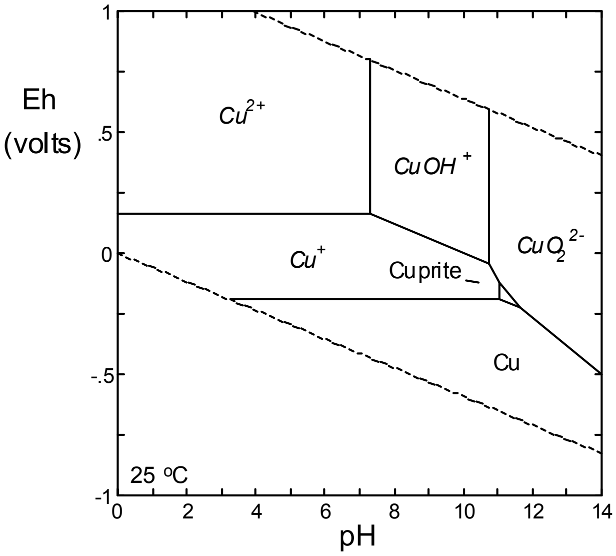

*Figure 4 Eh-pH diagram for copper (Cu concentration = $10^{-12}$ mol/l). Note the occurrence of the aqueous species $CuO_2^{2-}$ at pH >12, at relatively low Eh (-300 mV). Diagram constructed using Geochemists Workbench (Bethke, 1996).*

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# Simulation of Coupled T-H-M Processes in Engineering Barrier System For Disposal of Radioactive Waste and Spent Nuclear Fuel – A Review of DECOVALEX Project

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An important part of the performance and safety assessment of the disposal system for radioactive waste is to incorporate the coupling of mechanical stability, groundwater flow through the repository, and thermal loading from the decaying waste. To help meet these objectives and provide the theoretical background for performance and safety assessment, we aim to develop models capable of simulating coupled thermo-hydro-mechanical (T-H-M) processes. The term ′coupled processes′ implies that one process in the waste system affects the initiation and progress of the other. Thus, the response of the buffer or the backfill to decaying radioactive waste cannot be predicted with confidence by considering each process individually or in direct succession. In the field of rock mechanics, the main focus of studies has been on the binary couplings T-M and H-M. During the last decade, also corresponding to the time of the DECOVALEX project, the interest has been focused on the full triple T-H-M couplings. In the future, we can foresee the introduction of chemical processes (C) and, consequently, the study of T-H-M-C coupling.

Numerically, the coupled processes can be modelled by different techniques, such as finite-difference methods, finite-element methods and discrete-element methods. In addition, the considered processes in the canister-buffer-host rock are complicated with coupled, highly non-linear flow and deformation and vapour water flow, and the constitutive equations typically contain large parameter sets. To combine all these processes into an efficient model for the simulation of coupled T-H-M processes in fractured rocks is a difficult task.

Another aim for the study of coupled T-H-M processes is to be able to verify numerical codes and validate model results against well-designed and well-conditioned field and laboratory experiments. Here, the challenge lies in defining boundary conditions, rates of thermal and mechanical loadings, initial state of stress, temperature and flow, constitutive equations and material properties and to define and understand the variability and uncertainty of the results of the validation and verification.

The international project DECOVALEX (acronym for the international co-operative project for the DEvelopment of COupled models and their VALidation against EXperiments in nuclear waste isolation). The overall goal of the project is to increase our understanding of the various aspects of coupled T-H-M processes of importance in the release and transport of radionuclides from a repository to the biosphere and how mathematical models can describe these processes. The objectives of the DECOVALEX project can be summarized as:

- To support the development of computer codes for T-H-M modelling
- To investigate and to apply suitable algorithms for T-H-M modelling
- Compare theory and model calculations with results from field and laboratory experiments
- Design new experiments of coupled T-H-M processes for code development
- Develop and apply T-H-M modelling for performance and safety assessment

## DECOVALEX I

In the DECOVALEX I project that lasted 1992-1996, three hypothetical benchmark tests and three small laboratory tests of rock samples and joints and three large field tests were studied (Jing et al., 1995). One of the interesting benchmark tests simulated a Swedish KBS-3 disposal concept in a fractured granitic rock with the same fracture system and properties as the Stripa granite. The research teams were very successful in simulating the temperature distribution in the vicinity of the canister hole and the tunnel. The majority of research teams were also successful in predicting stress and displacement while the water flow was far from measured values. The discrepancies in flow of the hydro-mechanical system is fundamentally related to the unsatisfactory state of science of constitutive laws of rock discontinuities as well as the design of the conceptual models used at that time. Also most of the models of fractured rocks assume each of the fracture to have constant aperture and thus obey the so-called cubic law. However, it is well known that the aperture is strongly varying, giving rise to so-called channelling effect. In addition many of the basic parameters associated with the fundamental laws and with geometrical features of the fracture medium are not accessible for direct measurements.

## DECOVALEX II

In the second phase of the project – DECOVALEX II - it was decided to alter the focus to major large-scale in-situ experiments and to evaluate how the studies conducted in the project can be applied to the performance and safety assessment of a potential repository. The following studies were undertaken:

- Task 1: Numerical study of Nirex´s Rock Characterization facility (RCF) shaft excavation at Sellafield
- Task 2:Numerical study of T-H-M experiments in Kamaishi Mine, Japan
- Task 3: Review of the state-of-the-art of the constitutive relations of rock joints
- Task 4: Report on the current understanding of the coupled T-H-M processes related to design and performance assessment of radioactive waste repositories.

Results of Task 1, 2, and 4 are presented in Stephansson et al. (2001). Task 1 is unique in DECOVALEX to date in that an extensive data package about the geology, hydrology and rock mechanics was distributed to the research teams who were free to select, develop, and parameterize their own conceptual models of the Sellafield site. One particular outcome of the work in this task is the importance of prediction-calibration procedures in predicting the response to pumping and shaft sinking in this type of modelling. Another conclusion from the work under this task is the importance but also difficulty to perform the simulation as fully coupled processes.

The simulations of the Kamaishi Mine heater experiments have provided valuable experience in analysing coupled T-H-M analysis for problems similar to that proposed for a real waste repository. The results gave a true breakthrough in the simulation capacity of the complicated system of canister, compacted bentonite and saturated/unsaturated rock.

## DECOVALEX III

In the ongoing third phase of the project – DECOVALEX III – starting 1999 and ending 2003 the following tasks are performed:

- Task 1: Febex in-situ experiment in Switzerland
- Task 2: The Drift Scale Test (DST) in the Exploratory Studies Facility (ESF) at Yucca Mountain, USA

- Task 3:Three benchmark tests (a) Resaturation BMT1, (b) Homogenization BMT2 and (c) Glaciation BMT3.
- Task 4: T-H-M in performance assessment

Task 1

In the Febex experiment two large scale in-situ experiments are being performed: 1) an in-situ field test of heater-buffer-rock system with a long period of heating, followed by 2) a large scale laboratory "mock-up" test. The aim of the project is to demonstrate the present capabilities for building bentonite barriers in conditions similar to actual repository design and providing monitoring data to understand coupled THM processes in the near field. Large quantities of monitoring data regarding stress, deformation, water content, water pressure, and temperature distributions and their histories with time at a large number of monitoring places were recorded in-situ and a large number of rock/buffer property parameters were measured also in laboratory tests. Two sub-tasked are conducted within DECOVALEX III;
1) simulation of hydro-mechanical behaviour of the fractured rock mass with respect to the tunnel excavation; and 2) the simulation coupled thermo-hydro-mechanical responses of the complete rock-buffer-heater system during the whole heating period.

The first subtask requires predictions to the redistribution of water head field, flow rate field, stress field and deformation field in the rock mass induced by tunnel boring. The numerical models then can be supported and calibrated against monitored data on geological and hydrological characterization of the rock mass surrounding the tunnel, the hydraulic tests carried out before the tunnel excavation.

The second subtask requires predictions to responses of buffer and rock mass and their interactions, including temporal evolutions and spatial distributions of temperature, water content, water pressure, stress and deformation of the buffer material and rock mass near the tunnel. The results should be compared at selected points. As a global measure of the rock-buffer-heater system, the time history of the total system power input to the heater is also to be predicted. The prediction-calibration cycle can be maintained throughout the BMT to enhance the numerical capability and improve confidence.

Task 2

The Drift Scale Test (DST) in the Exploratory Studies Facility (ESF) at Yucca Mountain is a large-scale thermal test, conducted by the Yucca Mountain Site Characterization Office of the U. S. Department of Energy (DOE). It is part of DOE's program of characterizing the Yucca Mountain site to evaluate its suitability for a potential nuclear waste repository. The heating phase of the test, started on December 3, 1997, is scheduled to continue for approximately four years. The objective of the test is to help increase the confidence in models of coupled thermal-mechanical-hydrological-chemical processes in the rock mass. These models will be employed to quantitatively assess the long-term performance of the potential repository.

Heating is effected through nine cylindrical heaters placed on the floor of a 47.5 meter drift and 50 wing heaters, each 10 m long, inserted into horizontal boreholes into either side-wall of the drift. The purpose of this arrangement is to: (a) simulate the thermal pulse an emplacement drift will experience from its neighbours, and (b) heat a large volume of rock mass to boiling temperatures in a reasonable period of time. Measurements/monitoring made in the DST include is extensive.

DOE provides data to interested organizations in DECOVALEX III, who can use them to study and test the following kinds of codes and models:
1) Thermo hydrological (TH) codes: heat and fluid flow in unsaturated fractured rocks; heat pipe effect and other heat transfer mechanisms; effects of temperature dependence of permeability and conductivity, etc.

2) Thermo mechanical (TM) codes: changes in concrete lined drift; changes in the unsaturated rock; comparison between field and laboratory parameters (scale effect).
3) Thermo-hydro-mechanical (THM) codes: processes in unsaturated fractured rocks; including the presence of drifts; effects of thermo-mechanical processes on hydrologic characteristics.
4) Thermo-hydro-chemical (THC) codes: chemical changes under air-water-vapour flow in fractured rock; changes in Eh and pH; chemical reactions under phase change; effects of dissolution and precipitation on hydrologic characteristics.

Task 3
Task 3 consists of three benchmark tests BMT1, BMT2, and BMT3

BMT1
The resaturation BMT concerns with the resaturation of a hypothetical repository immediately after its closure and may be defined to include two alternative formations, fractured hard rock and sedimentary rock, to satisfy needs from different national waste repository concepts. The data bases developed at the FEBEX or the Monterri sites, both in Switzerland, may be used for the detailed technical definition of the BMT with alternative repository geometry. The main PA measures are the resaturation progress in buffer and rock, the mechanical effects on buffer and waste form, and the temperature distribution in buffer.

BMT2
The homogenisation BMT (as originally proposed as upscaling BMT) concerns the relationship between an equivalent continuum (which could be heterogeneous) and detailed discrete representations of fractured rocks, and the extrapolation of rock properties obtained from small scale test and observations to large repository scale, with analysis for uncertainties. The main PA measures are the methods of derivation of flow and deformation properties of the fractured rock from a small detailed model to large-scale equivalent continuum model, and its impact on large scale changes of flow and deformability fields. The database developed at Sellafield for the Task 1 of DECOVALEX II may be used for the detailed technical definition of the BMT.

BMT3
The glaciation BMT concerns mainly the hydro-mechanical impacts of a cycle of glaciation and deglaciation on the long term (up to 100,000 years) performance of a hypothetical post-closure repository, without considering the thermal effect. Many different scenarios could be included as alternative contents, such as permafrost, different ice-rock interface conditions, 2D - 3D transition, inland/coastal repository locations, sea level changes, saline water intrusion, fracture initiation, propagation and creeping, etc. The main PA measures will be the maximum deformation, changes of permeability fields, flow patterns and formation of critical flow paths, ground surface subsidence and rebound. Only long-lasting and large-scale changes in PA measures are significant. If a data set from SKB is used, the data set available for the project will be proposed by SKB and agreed upon by the Steering Committee of DECOVALEX III.

Task 4
In order to better understand the relevance of T-H-M coupling to performance assessment (PA), the associated uncertainties and the applicability ranges, the Task 4 is proposed as a platform for presentation, discussion and documentation on the treatment of T-H-M issues in the framework of PA analyses. The task contains two subtasks: i) Task 4a: a state-of-the-art review on the current and past international treatment of T-H-M issues in PA framework and ii) Forum and documentation on T-H-M treatment in the PA framework.

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Homepage for DECOVALEX III: www.DECOVALEX.com

# Interaction between the buffer material and the canister-

## - Preliminary analysis of geotechnical aspects

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## *Abstract*

The spent nuclear fuel and the radio active materials formed during the operation of the Swedish nuclear power plants will be enclosed into tight metal canisters. These canisters will then be placed in large disposal boreholes drilled into the floor of the repository tunnels. Bentonite blocks will be placed to fill the space between the canisters and the boreholes. The main purpose with the bentonite is to provide a hydrological barrier.

In general the types of analysis required to study the behavior of the canister and the buffer material shall account for mechanical, hydraulic, thermal and chemical effects. In this study, only near field mechanical behavior is investigated.

Preliminary analyses are made and presented, based on simplified assumptions and on some simple two-dimensional finite element solutions. As a result of the preliminary analysis, limited tectonical movements in the bedrock and unfavorable local swelling are studied and modeled by the finite element code ABAQUS using three-dimensional models.

The bentonite is modeled using two different material models, Mohr-colulomb and Drucker-Prager, while the canister materials are modeled using a Drucker-Prager material model.

A certain form of sensitivity analysis for parameters has also been carried out.

The analyses of uneven swelling of the bentonite did not give any plastic strains in the canister. Local swelling is therefore not a threat against the canister. This load case is not the critical one.

The results from the analyses of movements in the bedrock show that, as a consequence of large deviatoric stresses, plastic strains appear locally in the canister. However, the material properties for the materials in the canister show that the size of the deviatoric stresses is less than half on the failure stress. Thus, there seems to be no risk for local or total failure of the canister in case of movements in the bedrock.

The conclusion from the finite element analyses is that the design of the nuclear waste canister (KBS-3) is sufficient to protect the nuclear waste from mechanical load.

# A Summary of Key Technical Issues
# Related to Integrity of Engineered Barrier System

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## Introduction

This is an attempt to summarize key technical issues or questions concerning the integrity of engineered barrier system (EBS) and its role in the isolation of nuclear waste in a geologic repository. The collection of issues is extracted from discussions of the international DECOVALEX project, minutes of the SKI Near Field Meeting in Johannesberg and discussion topics of NEA-EC Workshop at Oxford in September 2002. While it is not expected to be complete, it hopefully can serve as a starting point to evaluate the state of art of the subject and to develop a strategy to work with SKB to ensure the optimal design of the EBS and proper modeling of its isolation behavior. The technical issues are listed below under a few main categories, after which some suggestions will be given for developing a possible strategy to conduct analysis and review of SKB's work.

## Bentonite Properties And Constitutive Equations

- Mechanical constitutive relationship for bentonite (e.g., "overheating" and irreversibility problems)
- Hydrologic characteristic equations for bentonite (e.g., potentially slow resaturation due to threshold gradient for Darcy flow and effect of micro-macro structure for bentonite)
- How are the properties of EBS components and the conditions under which they must function measured or characterized?
- Dependence of property parameter values on measurement techniques, such as sampling scheme, short-term laboratory measurements, and inferences from observation of natural systems.
- Evaluation of data inconsistencies and parameter uncertainties
- Are there scale effects on properties of various materials in the EBS (consistency between laboratory and field measurements)?

## Processes and Features

- Effects of evaporation and condensation (including the heat pipe effect) in the buffer rock system
- How to treat gas migration and its effects on EBS?
- Effect of buffer swelling or shrinking on canister over time (including uneven swelling)
- Effect of buffer swelling on nearby rock over time (including uneven swelling)
- Effect of diffusion-related couplings (Onsager couplings), such as Soret and Dufour effects, and thermal filtration and osmosis, in buffer-rock system under THM gradients
- Bentonite resaturation: effect of rock fractures, uneven wetting, locally tight rock, and also effect of bentonite dispersion when flushed by ground water, etc
- Postclosure resaturation-repressurization effects: potential reduction of effective stresses causing hydrofracturing with additional permeability changes in the near-field rock.
- Interaction among different materials in the waste, canister, bentonite, backfill, plugs and tunnel supports
- Processes and time dependent conditions at interfaces between waste form, canister, buffer, backfill, EDZ and rock

## Modeling

- Identification of basic assumptions and evaluation of their significance and impact on modeling correctness and accuracy
- How to define appropriate boundary conditions on models?
- What are the conceptual model and parameter uncertainties?
- Identification of model simplification or abstraction and evaluation of uncertainties introduced.
- Identification of connections between submodels and evaluation of uncertainties introduced
- Treatment of uncertainties and variabilities in heterogeneous geologic systems
- Need for modeling THM over different time scales?
- How to apply or use what we have learned from natural analogs?
- What have we learned from laboratory and subsurface field experiments of importance to modeling?
- How well are the models verified and validated, especially for results on 200,000 years time frame?

## Effects of Variability

- Variation of effects due to different locations within the repository

- Variability among canisters, such as different water contact times, different corrosion rates, different container/overpack failure and different rates of radionuclide releases, etc.
- How to evaluation human "errors", such as non-conformance of emplaced EBS, and variability of conditions for fabricaion and emplacement of canisters, etc.
- Effect of imperfect sealing at backfill boundary

### Effects of Repository Design and Construction

- What are the evolution of external condition (e.g., tectonic movements) over time?
- Impact on EBS system due to need to incorporate retrievability.in repository design
- Implication and opportunities for monitoring and performance confirmation; impact on EBS.
- Design of performance confirmation monitoring without affecting EBS mechanical integrity.
- Procedure for testing deposition holes and criterion for determining which holes are good for accepting waste canisters and which are not.
- Excavation disturbed zone (EDZ) around canister holes and drifts: how to characterize it and how to evaluate their impact on safety?
- Significance of tunnels on safety assessment.
- Impact on EBS due to measures taken to maintain stability and reduce water inflows
- What are the changes in stress and hydraulic conditions and fluxes at excavation, canister and buffer emplacement, backfill, closure and sealing.
- Evolution of conditions over time; impact of repository development, such as excavation methods, duration of operation prior to closure.
- Repository-induced influences over time on the EBS and its performance Impact of varying conditions around EBS on its role in radionuclide transport
- Geochemical (including pH and redox) conditions in the near-field environment
- Transient behavior of EBS during initial stage with large changes and large gradients in temperature, moisture etc.

### Analysis and Review Strategy

The list of technical issues or questions above serves as a reminder of some of the important processes or conditions that need to be considered, investigated and understood, in order to be assured of the integrity of the EBS and its isolation function in a geologic repository. For each topic, it may be useful to

(a) discuss its role in repository performance and its importance to safety assessment,
(b) decide if current state of art is mature or weak
(c) suggest approach that SKI should take regarding to this topic (ranging from paper review, simple verifying scoping calculations, to parallel analyses).

In developing a strategy for analysis and review, it may be useful to consider the following questions

- SKB’s so-called “base scenario” may not be a realistic or typical scenario of main interest for SKI’s review; how to define a scenario of focus for SKI?
- What are the urgent issues versus those that can be addressed later? Can we develop a list of questions or requests to SKB with a time schedule over the next months and years?
- Should we request now the property values from SKB, especially those of the backfill and repository materials, such as bentonite, concrete, rock bolts etc?
- Should we request now SKB’s documentation on codes to be used for license application to ensure their verification, transparency and traceability
- Should we review now SKB’s codes (some may be well known and require little effort, but others may not)?
- What are the lessons learned from major URL’s, such as Aspo in Sweden, Febex in Switzerland, Kamaishi in Japan, etc.
- When and how to conduct Structured Expert Elicitation?
- What is the role and use of natural analog studies?