Strål
säkerhets
myndigheten
Swedish Radiation Safety Authority

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Technical Note

2012:18

SR-Site Independent Modelling of Engineered Barrier Evolution and Coupled THMC: Contribution to the Initial Review Phase

Report number: 2012:18 **ISSN:** 2000-0456
Available at www.stralsakerhetsmyndigheten.se

SSM perspektiv

Bakgrund

Strålsäkerhetsmyndigheten (SSM) granskar Svensk Kärnbränslehantering AB:s (SKB) ansökningar enligt lagen (1984:3) om kärnteknisk verksamhet om uppförande, innehav och drift av ett slutförvar för använt kärnbränsle och av en inkapslingsanläggning. Som en del i granskningen ger SSM konsulter uppdrag för att inhämta information i avgränsade frågor. I SSM:s Technical note-serie rapporteras resultaten från dessa konsultuppdrag.

Projektets syfte

Syftet med denna rapport är att granska SKB:s arbete med integrerad modellering av hur det tekniska barriärssystemet utvecklas samt att genomföra begränsade egna oberoende modelleringar/beräkningar. Utvecklingen av THMC egenskaperna för buffert och återfyllnadsmaterial och korrosion av kopparkapseln ska granskas med hänsyn till hur buffertens egenskaper såväl som hur randvillkoren med avseende på grundvattenkemi och grundvattenflöden kan förändras med tiden. I denna inledande del av granskningen är målet att identifiera behovet av vilken kompletterande information som SKB bör lämna till SSM inför nästa fas av granskningen.

Författarnas sammanfattning

Denna granskning har huvudsakligen fokuserats på hur det tekniska barriärsystemet (EBS) utvecklas med tiden med avseende på följande samverkande (THMC) processer termiska, hydrauliska, mekaniska och kemiska. Dessutom har de tekniska barriärerna granskats i ett bredare säkerhetsredovisningsperspektiv med avseende på hur barriärerna behandlas i scenarieanalysen samt i konceptuella modeller eftersom att detta är grunden till hur SKB arbetat med modeller. Omfattningen av arbetet i denna rapport var att:

- Granska relevanta dokument med avseende på hur SKB modellerat utveckling av tekniska barriärer.
- Kontrollera utgående från granskningen ett utvalt modelleringsområde som anses speciellt viktigt med en begränsad egen oberoende modellering/beräkning.

Granskningen innefattar återmättnadsfasen och svällning/homogenisering av bufferten, den långsiktiga kemiska utvecklingen av buffert och återfyllnadsmaterial, korrosion av kopparkapseln och de kemiska och hydrogeologiska randvillkoren som ges av det omgivande berget.

Granskningen visar att SKB:s modellering av de tekniska barriärernas prestanda i huvudsak stödjer deras slutsats att de tekniska barriärerna kommer att uppföra sig efter uppställda behov. Det finns emellertid kvarvarande frågor och osäkerheter i SKB:s modellering som inte besvarats i tillräcklig omfattning.

SKB:s termo-hydro-mekaniska modellering av buffertens återmättnad baseras på anpassning till mätdata från "Canister Retrival Test (CRT)" försöket. SKB:s modellering reproducerar några experimentella iakttagelser mycket bra medan andra experimentella resultat som anses speciellt viktiga inte har beaktats. I detta sammanhang bedöms att anpassning av uppmätta hastigheter av vattenflöde in till bufferten till beräkningsmodellen inte ha redovisats, vattenflöde in till bufferten är en kritisk faktor som kontrollerar hur snabbt bufferten återmättas. Dessutom anses att det sätt som vatten tillförts till bufferten i CRT experimentet inte vara representativt för de förhållanden som gäller i det planerade slutförvaret. Från SKB:s redovisning är det därför inte möjligt att bedöma dugligheten i SKB:s modeller att förutsäga realistiska inflödeshastigheter av vatten eller hur återmättnaden av bufferten sker under förväntade förhållanden i slutförvaret där återmättnad sker via vattenflöden från sprickor i berget. Ytterligare experimentellt och modelleringsarbete bör utföras.

Kemisk förändring av buffertmaterialet behandlas på ett inkonsekvent sätt i säkerhetsredovisningen. För växelverkan mellan grundvatten och bentonit används modeller som bygger på termodynamisk jämvikt medan för att beskriva växelverkan mellan cement och bentonit så används kinetiska modeller som bättre beskriver den sanna kemiska förändringsprocessen. Känsligheten av den rumsliga diskretiseringen som beskrivs i modellerna vilka kan leda till olika beräknade tider för igensättning av porositeten med omvandlingsprodukter diskuteras inte. Där kinetiska modeller används, tas lite hänsyn till osäkerheter i reaktionshastighet för mineralomvandlingar, vilket kan ha stor påverkan för den predikterade utvecklingen av det undersökta systemet.

Beräkningar av kopparkapselns korrosionshastighet beroende på ämnen i grundvattnet som påverkar korrosionen av kapslarna ger ett konservativt resultat för den valda grundvattenflödesgeometrin, emellertid är den valda geometrin inte nödvändigtvis konservativ för andra geometrier. Egna begränsade beräkningar antyder att korrosionshastigheten kan ske snabbare för andra valda grundvattenflödesgeometrier. Ytterligare modelleringar bör utföras för att undersöka inverkan av grundvattenflödesgeometri på korrosionshastigheten och även för att kontrollera konservatismen och noggrannheten av de förenklingar som används av SKB i deras korrosionshastighetsberäkningar.

Dokumentation av det sätt på vilket EBS tas om hand i säkerhetsredovisningen och hur det tas om hand i modellerna är ofta oklart och svårt för läsare att följa. Av denna anledning är det svårt att med säkerhet fastslå vilken kvalitet som de använda modellerna har.

Projektinformation

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Diarienummer avrop: SSM2011-4208
Aktivitetsnummer: 3030007-4010

SSM perspective

Background

The Swedish Radiation Safety Authority (SSM) reviews the Swedish Nuclear Fuel Company's (SKB) applications under the Act on Nuclear Activities (SFS 1984:3) for the construction and operation of a repository for spent nuclear fuel and for an encapsulation facility. As part of the review, SSM commissions consultants to carry out work in order to obtain information on specific issues. The results from the consultants' tasks are reported in SSM's Technical Note series.

Objectives of the project

The objectives of this work are to address SKB's integrated modelling of engineered barrier evolution through review efforts and a limited set of independent modelling/calculations. The THMC-evolution of the buffer and backfill shall be addressed as well as the corrosion of the copper canister considering the evolution of the buffer as well as the basic boundary conditions provided by the bedrock in terms of groundwater chemistry and flow conditions. In this initial review phase the aim is to identify the need for complementary information and clarifications to be delivered to SSM by SKB.

Summary by the authors

This review has focussed mainly on the modelling of the Engineered Barrier System (EBS) evolution, which includes coupled thermal, hydraulic, mechanical and chemical (THMC) processes. Additionally, the role of the EBS in the wider safety case was reviewed, including its treatment in scenarios and its representation in conceptual models since this provided the motivation for the modelling work that was undertaken by SKB. The scope of the work described here was to:

- Review relevant documents concerning SKB's modelling; and
- Check one particular modelling area that was judged to be important, based on this review, with a limited set of independent modelling/calculations.

The review covers the early resaturation and swelling / homogenisation of the buffer; the longer-term chemical evolution of the buffer and backfill, corrosion of the copper canister and the chemical and hydrogeological boundary conditions provided by the surrounding host rock.

The reviewers consider that SKB's modelling of engineered barrier performance generally supports their conclusion that the barriers will perform as required. However, there remain issues that are not addressed and uncertainties that are not explored adequately by SKB's modelling. The thermo-hydro-mechanical modelling of buffer resaturation that is performed by SKB is based on demonstrating a fit to measurements from the in-situ Canister Retrieval Test (CRT) experiment. The modelling reproduces some of the experimental observations very well, but some key experimental measurements are not considered. In particular, investigation of the fit to the measured rates of water inflow, which are a critical factor controlling the rate at which the buffer will resaturate, is not given, Furthermore, the water supply boundary conditions imposed on the CRT are not considered to be representative of those that might be expected in repository conditions. From the information that it is presented it is therefore not possible to be confident in the ability of SKB's models to predict realistic rates of inflow, or patterns of resaturation in the buffer, that might be expected under true repository conditions when resaturation arises from flows in small fractures. Further experimental and modelling work should be performed.

Chemical alteration of the buffer is treated inconsistently in the safety case. Thermodynamic equilibrium models are used to simulate groundwater-bentonite interactions whilst kinetic models, which better reflect the true chemical alteration processes, are used to simulate cement-bentonite interactions. Sensitivity to the spatial discretisation that is considered in the models, which can lead to different computed timescales for clogging of porosity with alteration products, is not discussed. Where kinetic models are used there is little consideration of the underlying uncertainties in mineral reaction rates, which can greatly affect the predicted evolution of the system.

Calculation of rates of corrosion of the copper canister due to corrodants in the groundwater, though conservative for the particular groundwater flow geometry employed, are not necessarily conservative for other flow geometries. Scoping calculations suggest that faster rates of corrosion are possible in some cases. Further work should be performed to investigate this sensitivity and also to check the conservatism and accuracy of simplifications in SKB's corrosion rate calculations.

Documentation of the way in which the EBS in considered in the safety case and its representation in models is often unclear and difficult for readers to follow. Consequently, it is hard to form firm conclusions about the quality of the modelling.

Project information
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Technical Note 5

2012:18

SR-Site Independent Modelling of Engineered Barrier Evolution and Coupled THMC: Contribution to the Initial Review Phase

Date: June 2012
Report number: 2012:18 **SSN:** 2000-0456
Available at www.stralsakerhetsmyndigheten.se

Content

1. Introduction

The Swedish Radiation Safety Authority, Strålsäkerhetsmyndigheten, (SSM) is reviewing the SR-Site safety assessment, which was undertaken by the Swedish Nuclear Fuel and Waste Management Company (SKB). The purpose of the SR-Site safety assessment was to support SKB's licence application for a final spent nuclear fuel repository at Forsmark. This report is a contribution to the Initial Review Phase of SSM's review.

This review has focussed mainly on the modelling of the Engineered Barrier System (EBS) evolution, which includes coupled thermal, hydraulic, mechanical and chemical (THMC) processes. Additionally, the role of the EBS in the wider safety case was reviewed, including its treatment in scenarios and its representation in conceptual models since this provided the motivation for the modelling work that was undertaken by SKB. The review covers the early resaturation and swelling / homogenisation of the buffer; the longer-term chemical evolution of the buffer and backfill, corrosion of the copper canister and the chemical and hydrogeological boundary conditions provided by the surrounding host rock.

The high level structure of this report is as follows: the overall aims and approach taken for this review are described in the remainder of this section; Section 2 and Section 3 list the main review findings and recommendations to SSM; Section 4 contains details of the review of the modelling of the EBS, and provides more details on the review findings and recommendations; Section 5 contains scoping calculations that were performed to investigate issues that arose during the review; and Section 6 describes independent modelling that has been performed to review the ability of THM models to reproduce resaturation behaviour that has been observed in in-situ experiments and discusses the applicability of such models to modelling resaturation under in-situ conditions. Appendix 1 lists the SKB reports that have been consulted during this review with an indication of the degree of coverage that has been achieved; Appendix 2 provides a list of complimentary information that should be requested from SKB and questions that should be raised; and Appendix 3 lists some review topics that are suggested for the main review phase. Appendix 4 provides some detailed review comments on specific statements made in the reports that have been consulted.

1.1. Background and Aims

The Initial Review Phase aims to develop a broad understanding of the SR-Site assessment and its supporting modelling studies. In particular this initial phase aims to identify the need for complementary information and clarifications to be delivered by SKB. This contribution concerns SKB's modelling of engineered barrier system (EBS) evolution and coupled thermal, hydraulic, mechanical and chemical (THMC) processes. The scope of the work described here was to:

- Review relevant documents concerning SKB's modelling; and
- Check one particular modelling area that was judged to be important, based on this review, by means of a limited set of independent modelling/calculations.

The review covered corrosion of the copper canister, the evolution of the buffer and backfill and the chemical and hydrogeological boundary conditions provided by the surrounding host rock.

After the Initial Review Phase has been completed, SSM will determine if the quality and comprehensiveness of the safety assessment SR-Site is sufficiently good to warrant the planned in-depth assessment during the Main Review Phase of the licence for construction, possession and operation of the spent nuclear fuel repository in Forsmark. In the Main Review Phase following the Initial Review Phase, SSM will identify uncertain and/or safety critical review issues that require a more comprehensive treatment and initiate more detailed modelling studies to achieve and in-depth understanding of issues that are critical for long-term safety.

1.2. Approach to Review

This contribution to the Initial Review Phase was undertaken in a “top-down” fashion. That is, the review started by considering general topics and developed through several steps to consider progressively more detailed topics. Each step focussed on more detailed aspects of any issues identified in the previous step. The following activities were undertaken in order:

1. review representation of EBS evolution in scenarios (Section 4.2);
2. review, the conceptual models of EBS evolution that are represented in these scenarios (Section 4.3);
3. evaluate representations of these conceptual models in numerical models of EBS evolution (Section 4.4).
4. review computer software used by SKB to implement the numerical models of EBS evolution (Section 4.5);
5. review data used to carry out the numerical models of EBS evolution (Section 4.6).
6. carry out scoping calculations out to check key aspects of SKB’s numerical models of EBS evolution (Section 5).
7. carry out detailed coupled modelling to check a key aspect of SKB’s numerical modelling of EBS evolution that was judged to be particularly significant (Section 6).

The review focussed on technical issues. Typographical and grammatical errors that could lead to these technical issues being misunderstood by a reader were also covered. Other such errors, which affect the presentation rather than the substance of the issues covered, were not recorded in detail. However, examples of these kinds of error are given and recommendations made for correcting them.

All the documents consulted during these activities, and the nature of the reviews to which they were subjected, are listed in Appendix 1. In summary, reviewed documents are:

1. SKB reports indicated by SSM to be a mandatory subject of the review:
    - TR-11-01: Main report of the SR-Site project;

    - TR-10-51: Model summary report for the safety assessment SR-Site;

    - TR-10-52: Data report for the safety assessment SR-Site.

2. SKB reports indicated by SSM to be relevant to the review::

    - TR-10-66: Corrosion calculations report for the safety assessment.

    - TR-10-11: THM modelling of buffer, backfill and other system components. Critical processes and scenarios.

    - TR-10-59: Aspects of geochemical evolution of the SKB near field in the frame of SR-Site

3. SKB reports that were identified as containing relevant information during the course of the view.

2. Main Review Findings

Summary findings of the review are presented in Table 1, which covers the general topics listed in the review guidelines provided by SSM.

Table 1 Independent modelling of engineered barrier evolution and coupled THMC: summary of findings

Issue	Finding
Completeness	**Inadequate**: SR-Site has covered a wide range of calculation cases for the buffer and backfill, but its completeness is considered "Inadequate" because some aspects have not been considered and there are inconsistencies in the arguments presented. For example: • Models used in predicting timescales for resaturation of emplaced buffers have not been demonstrated to reproduce measured experimental inflow rates. Experimental observations suggest that heterogeneous resaturation patterns may exist in the bentonite for long periods, but this has not been covered adequately in SKB's reports. • It has not been established that corrosion is modelled conservatively. • The approach to reactive transport modelling is inconsistent. Thermodynamic equilibrium approaches are used for groundwater-bentonite modelling and kinetic approaches, which more realistically represent the chemical alteration processes are used for cement-bentonite modelling. In each case, key uncertainties (e.g. of kinetic rates) and sensitivities (e.g. to grid resolution) in the models are not discussed or explored. **Recommended Action** SSM should require additional numerical analysis to cover gaps and to assess the significance of inconsistencies in the arguments presented. For more detailed recommendations see Section 3.

Scientific soundness and quality	**Apparently Good**: Here the scientific soundness and quality are considered to be “Apparently Good” because all scientific methods and arguments are considered reasonable, but the way in which SKB presents its modelling in the **main report of the SR-Site project** (TR-11-01) and supporting documents is not always clear and tends to obscure quality-relevant information. Therefore, we cannot be completely confident in our conclusion. **Recommended Actions** Through the future review programme, SSM should seek to build more confidence in the scientific soundness and quality of the safety assessment work. As a first step, To improve the quality of transparency and traceability of information, SSM could request that SKB prepare a complete, concise and more transparent data report, that contains all the data / information used in the assessment (see Section 3.1for more detailed recommendations). This action should be accompanied by more detailed review of specific topics. .
Adequacy of relevant models, data and safety functions	**Generally good:** Here the adequacy of the relevant models, data and safety functions are considered to be “Generally Good” because these give a large degree of support to the main arguments concerning safety, but there are inconsistencies in the details of some models and supporting experiments, principally: • Coupled models of buffer resaturation (e.g. **THM modelling of buffer, backfill and other system components**, TR-10-11) do not adequately reproduce resaturation measurements in the Canister Retrieval Test (CRT) that was undertaken by SKB at Äspö. • The boundary conditions considered in this experiment are not representative of those that might be expected under in-situ conditions, yet no other boundary conditions are considered in the detailed THM modelling. • Calculations of corrosion in **the corrosion report** (TR-10-66) though conservative for the particular groundwater flow geometry employed, are not necessarily conservative for other flow geometries, e.g. when fractures are assumed to intersect the buffer in locations other than the canister mid-height. • Models of cement evolution and cement-bentonite interactions (reports on **evaluation of low-pH cement degradation**, TR-10-62 and **quantitative modelling of cement degradation processes,** TR-10-25) produce results that are highly dependent upon the spatial discretisation used and the choice of kinetic reaction rates. The predicted limited extent of reaction partly depends upon this discretisation. **Recommended Action** SSM should require additional numerical analysis to address inconsistencies in models and supporting experiments. For more detailed recommendations see Section 3.

Handling of uncertainties	**Generally good**: Here the handling of uncertainties is considered to be "Generally Good" because the treatment gives a large degree of support to the main arguments concerning safety, but the analysed uncertainty ranges do not demonstrably cover the ranges of uncertainties in realistic system behaviours. At a high level, the range of calculation cases that have been evaluated allow the investigation of conceptual, model and data uncertainties using both deterministic and probabilistic approaches, but: • Conceptual uncertainties regarding flow geometry appear to not be represented in the corrosion calculations, resulting in incorrect conservative estimates. • Uncertainties in thermodynamic and kinetic data have not been considered in cement-bentonite modelling. • Realistic boundary conditions have not been applied to THM models of buffer resaturation. **Recommended Actions:** SSM could require updating of the analysis of uncertainties related to corrosion (see Sections 3.3 for more detailed recommendations) and to geochemical modelling (see Sections 3.5 and 3.6 for more detailed recommendations). SSM could ask SKB to continue their modelling of bentonite homogenisation to investigate boundary conditions that are more consistent with likely in-situ conditions at Forsmark.

Safety significance	**Possibly Significant**: Here, the issues that have been covered by the review are considered to be "Possibly Significant" because they concern system components that have been assigned important safety functions, but at this stage the actual significance of the identified issues is unclear. The safety of the repository depends mainly on: 1. the number of canisters that fail; 2. the time of failure; 3. the fuel dissolution rate; 4. the advective travel time; and 5. the transport resistance along the geosphere flow path. The present review covers canister corrosion and long-term modelling of buffer and backfill materials and is therefore relevant to items 1 and 2. The review has found that SKB's modelling of the barrier components has bounded the effects of all plausible barrier evolutions, for example by analysing an appropriate range of scenarios. However, SKB's modelling of buffer resaturation and corrosion is not adequately realistic and SKB's modelling of corrosion appears to contain errors in conservatism. The present review has not established the potential significance of these inadequacies for overall safety. **Recommended Action:** To determine the safety significance of the identified issues, SSM could require additional numerical analysis to be carried out as part of the main review phase. See Section 3 for more detailed recommendations.

Quality in terms of transparency and traceability of information	**Poor**: The quality in terms of transparency and traceability of information is considered to be "Poor" because information relevant to the coupled modelling of engineered barrier components is dispersed through numerous reports rather than being summarised in a single high level report that then references supporting detailed reports. All the reports need to be read to develop an understanding of the approaches used. Transparency and traceability is further hindered by the reports often not citing section numbers when other SR-Site reports are referenced. A particular deficiency is the poor reporting of data used in SKB's modelling of the engineered barrier components. These data are not presented in a single source and those sources that do present the data (e.g. the **buffer production report** (TR-10-15), the **backfill production report** (TR-10-16) and the **data report**, TR-10-52) obscure the data that were actually used in SKB's modelling by also giving lots of information concerning the means by which the data were obtained. **Recommended Action:** To improve the quality of transparency and traceability of information, SSM could request that SKB prepare a complete, concise and more transparent data report, that contains all the data / information used in the assessment. In future, SSM should require SKB to produce such complete and concise documentation. For more detailed recommendations see Section 3.1.

Generally, the English of the reviewed documents is understandable but there are numerous grammatical expressions that would not be used by a native English speaker and some of these expressions are potentially confusing. Also, in many of the supporting documents there are several typographical and grammatical errors. Some typographical and linguistic errors are unavoidable in an extensive and complex set of documents like those reviewed in the present report. However, the large number of such errors is surprising in a suite of documents that is intended to support a license application and to be subjected to international peer review.

The structure of the **main report of the SR-Site project** (TR-11-01) is difficult to follow, with the same topics being covered at various levels of detail at different times, but often without adequate cross-referencing between them. While some sections include many cross-references, this is not always the case. For example, the last paragraph on page 71 of volume 1 of TR-11-01 concerns the main scenario and states that this scenario is based on the reference evolution. However, there is no cross-reference to the detailed description of the reference evolution in Section 10 of TR-11-01, commencing on page 287, which is in volume 2. Similarly, the paragraph on page 71 gives no cross-reference to the description of the main scenario analysis in Section 12 of TR-11-01, starting on page 571, which is in volume 3. Such cross-referencing would greatly enhance a reader's ability to appreciate how the assessment was undertaken and to understand the results.

Cross-referencing of source documents in TR-11-01 is also frequently inadequate. In many cases justifications for important conclusions are not given directly, but instead a reference to another report is given. Furthermore,. it would be helpful for cross references to be given unambiguously in the form "SKB, 19XXa" or "report TR-XX-YY". In fact, TR-11-01 usually provides cross references to supporting documents in the form an abbreviation of a report's title, for example "the SR-Site data report", "the canister production report" or "the buffer, backfill and closure process report". Potentially, this approach to referencing could lead to some confusion, since several supporting reports have superficially similar titles.

The **main report of the SR-Site project** (TR-11-01) contains many examples of subjective judgements that are not well-explained or supported by evidence. For example, page 158, para 6, line 6 states that "It is, however, assessed as justified to assume that very large and very transmissive fractures would be detected". While statements of this kind may well be reasonable, some more supporting evidence should be given.

It is impractical to list all the typographical and linguistic errors that were identified in the review. However, examples are given here:

- Page 360 para 5, line 5 of TR-11-01 refers to "organic *gunge* and biofilm". "Gunge" is not a usual technical term. "organic *gunge*" is also referred to on Page 23, paragraph 9, line 5 of the **corrosion report** (TR-10-66).
- Page 393, para 1, line 6 of TR-11-01 states that "Similarly to a process of loss of dolomite, secondary calcite precipitates in the Ibeco RWC bentonite". This sentence is awkward English and its literal meaning is not the one intended since it states that dissolution and precipitation are similar processes.
- Page 395, paragraph 10, line 5 states that "Thus, potassium is a must for the montmorillonite to turn into illite.". This sentence would be appropriate for a spoken presentation, but is not usual written English in technical documents.

The treatment of the EBS in the scenarios defined in the **main report of the SR-Site project** (TR-11-01) covers all potential failure modes of the buffer and canisters. However, the description and classification of scenarios is confusing. For example, the main scenario is based on a defined reference evolution and includes canister failure by corrosion. However, there is a separate "additional scenario" for canister failure by corrosion and the two are not clearly distinguished; it is easy for the reader to become unsure about whether canister corrosion is being treated as part of the main scenario or as a distinct scenario. Additionally, the distinction between "less probable" scenarios and "residual scenarios" and the rationale for the distinction is unclear.

The modelling of EBS evolution and coupled THMC processes that support the **main report of the SR-Site project** (TR-11-01) are described in the **THM modelling report** (TR-10-11). This modelling is impressive and of a high standard although there is little discussion of the performance implications of the modelling results.

Overall TR-10-11 is presented as a collection of independent modelling exercises using different codes and models. There is obviously a lot of overlap and inter-relation between the various sections, for example between the buffer resaturation modelling section (Section 3) and the section on buffer homogenisation (Section 5). However, there is very little cross-referencing within the report to establish these connections. The reader is left with the impression that 'lessons learned' in one modelling exercise are not being taken advantage of in others. For example the THM models that were developed for the homogenisation study are presumably better models of resaturation than the TH models that were used to make predictions of the time taken to resaturate the buffer and backfill under different assumptions. A THM model (referred to as "THM CRT") is used to calibrate the TH models but details of the THM model are given and no reference to more information is provided.

The referencing back to data sources in TR-10-11 is very poor. Model parameter values are introduced with no explanation and the reader is left unsure whether these values arise from measurements, modelling best fits or expert guesses. Similarly, equations, including constitutive equations, are introduced in the report with no reference to explanatory texts and often without any description of the terms appearing in the equations or their units. The non-expert reader would most likely find these aspects of the report impenetrable, which detracts from the modelling, which is of a high standard.

Radionuclide transport is outside the scope of this review. However, transport of solutes that could participate in chemical reactions within the buffer and backfill, or corrosion of the canisters, is relevant to modelling long-term EBS behaviour. Consequently, transport parameters reported in the **data report** (TR-10-52) were reviewed. Section 1.1 of this report states that: "This report compiles, documents, and qualifies input data identified as essential for the long-term safety assessment of a KBS-3 repository…". However, the document does not contain all the data that is required for transport calculations, while describing the data that are included at variable levels of detail. For example, little information is given about the compositions of the buffer and backfill materials. Instead readers who seek detailed information are referred to the **buffer production report** (TR-10-15) and the **backfill production report** (TR-10-16). In contrast, in Section 5.3 of TR-10-52 there is a highly detailed description of the approach to selecting Kd values in buffer and backfill materials. Furthermore, the detailed descriptions of the approach for selecting Kd data for the assessment are presented in a very complex and often unclear way which is difficult for the reader to follow, thereby making it difficult for them to form an opinion about data quality.

In Sections 5.3.5, 5.3.6 and 5.3.7 of TR-10-52 many uncertainties are raised in the mind of the reader because the stated assumptions and / or rationale for making choices among different data sets are not well-justified. In many places "proposals" are made for selecting data, leaving the reader to wonder what was actually done in the assessment. It would have been more appropriate to clearly specify values for use in the assessment and then discuss their associated uncertainties.

An important omission from Section 5.3.6 of TR-10-52 is a discussion of the nature and validity of the Kd concept and the limitations on its application.

Section 5.3.7 of TR-10-52 concerns the data uncertainties due to precision bias and representativity. However, again assumptions are often not clearly explained. Furthermore in some places data are recommended to precisions that are not really justified given the overall uncertainties. This is the case for diffusivities. In other places very broad statements are made about uncertainties without explaining their significance. For example, page 165 gives best estimate De values of 1.4×10^{-10} m^2/s for the buffer ($\rho d = 1{,}562$ kg/m^3) and 1.6×10^{-10} m^2/s for the backfill ($\rho d = 1{,}504$ kg/m^3)". Given that the difference between these values is small compared to the large scatter in the De data shown in Figure 5-6, it is unjustified to recommend different values for the backfill and the buffer. On the other hand, on page 168 the first paragraph of the section entitled "Diffusion-available porosity" reports that published diffusion-available porosities for Cl are a factor of 1.8–3.5 smaller than for HTO. It is then proposed to use a reduction factor of 2.5 based on these data. However, the arithmetic mean of 1.8 and 3.5 is 2.65. Hence, why was a value of 2.5 recommended? While perhaps a minor issue, this case illustrates the inconsistent approaches adopted in this report when recommending parameter values for use in the assessment.

3. Recommendations to SSM

In this section, recommendations for activities for the main review phase are given to SSM, together with some general recommendations that may help to simplify future iterations of the review. General recommendations are given in the first subsection that follows, with subsequent subsections providing recommendations in each of the main modelling areas that have been considered in the review. The justification for these recommendations is provided in individual review topics considered in Section 0.

3.1. General

1. It is recommended that SSM should encourage SKB to prepare its future reports of safety assessments and supporting activities in a standardized format. This format should enhance the ability of readers to trace the origins of information and the justifications of the arguments that are made.

2. It is also recommended that SSM should request SKB to prepare a single report of all the data and information that was actually used in the SR-Site assessment. This report should include *all* the data actually used by SKB when modelling the EBS system. While the document should indicate uncertainties in the data, detailed discussion of the means by which the data were obtained are not needed. Rather references to the relevant documents should be given.

3.2. Modelling Resaturation and Swelling / Homogenisation

1. Independent models that aimed to mimic SKB's models failed to represent the 'self-sealing' behaviour that was observed in the measured CRT data. Cumulative inflow data should be presented for SKB's THM models of the CRT and compared to the measured CRT data to see if they also fail to represent this behaviour.

2. Further THM modelling should be undertaken to improve the representation of the competing suction and permeability relationships as saturation varies within the bentonite. These new models should be carried out in 2D and should focus on more adequately accounting for observed full-scale resaturation in the CRT.

3. After demonstrating that the CRT inflows can be adequately represented, additional modelling should be undertaken to determine the change in the response to resaturation in the buffer when more realistic in-situ boundary conditions are applied. The modelling should investigate the plausibility and implications for buffer performance of long-lived heterogeneous buffer resaturation patterns. This modelling should be carried out in 2D and ideally would take into account chemical processes that will affect the buffer. Inclusion of chemical processes should enable investigation of the consequences of combinations of potentially less favourable groundwater chemistry in combination with potentially less favourable fracture geometries. For example, the modelling should investigate the potential consequences of water with salinity near the lower plausible limit, flowing

through an essentially 1D channel in a fracture that intersects a deposition hole near the top of a canister.

4. The MX80 and Ibeco bentonites are presented as being interchangeable in SR-Site, but their hydro-mechanical performance could in fact be dissimilar. Ibeco bentonite has a monovalent: divalent cation ratio of around 1:3, whereas in MX80 the ratio is 4:1, and so hydro-mechanical properties could be quite different (see e.g. Cui et al., 2011) .The modelling presented in TR-10-11 is only performed for the MX80 bentonite. Resaturation and swelling/homogenisation models calibrated for Ibeco bentonite should also be run.

5. It would be appropriate for SKB also to investigate the results from the FEBEX experiments at Grimsel and to develop models that can reproduce these results. The FEBEX experiment behaved differently from the CRT at Äspö. If models could be developed to reproduce the results from both tests, then confidence in the understanding of buffer resaturation would be improved. The FEBEX bentonite is perhaps closer in composition to the Ibeco bentonite than MX80.

6. Potential hydrogeological interactions between neighbouring deposition holes should be investigated. For example, in a slow flowing fracture, the possibility for an ‘upstream’ deposition hole to draw water towards itself and deprive downstream deposition holes of water should be investigated. This could have the effect of reducing hydraulic heads below hydrostatic for long periods at fracture intersections with downstream holes.

3.3. Modelling Corrosion and Erosion

1. Independent calculations should be performed to:

    - validate the distribution of corrosion rates calculated by SKB, in particular to check that the Q_{eq} transport terms are sufficiently accurate or that the resulting transport rates are conservative;

    - check that simplifications and assumptions made in the derivation of Q_{eq} terms do not lead to inaccuracies when different geometrical configurations are assumed; and

    - check the use of the Buffer Concentration Factor (BCF), to confirm whether or not it underestimates the likely amounts of corrosion when fractures are located away from the canister mid-height (as is suggested by independent calculations) and / or are combined with spalling and unfavourable flow conditions.

2. Arguments should be developed, supported by mechanistic calculations, to justify, or better understand the likely erosion geometries that might occur. The calculations should investigate the sensitivity of erosion to the location of the fracture(s). This would help to determine whether the corrosion areas that are suggested are truly based on conservative assumptions. In particular it should be clarified whether the assumption of a constant

growth rate on a semicircular cross-section of the eroded volume refers to the radius or the area of the cross section.

3. The **corrosion report** (TR-10-66) and literature that supports it should be reviewed more thoroughly than was possible during the initial review reported in this document. The detailed review should focus on uncertainties in mathematical treatment of corrosion/erosion that were identified in this initial review. An assessment should be made of the implications of these uncertainties for the calculated probabilities of canisters experiencing corrosion over the full depth of the copper casing during the 1,000,000 y assessment period.

4. The bentonite erosion mass transport model used in the corrosion calculations described in the **corrosion report** (TR-10-66) should be checked by reviewing the report **on mechanisms and models of bentonite erosion** (TR 09 35) and the report **on modelling of erosion of bentonite gel by gel/sol flow** (TR 10 64).

3.4. Modelling Geosphere / EBS Interface

1. The conceptualisation of fracture flow paths and their intersections with deposition holes, which underpins models of buffer resaturation in the **main report of the SR-Site project** (TR-11-01), needs to be reviewed in detail. The aim of the review would be to establish how alternative conceptualisations might influence the modelled resaturation of the buffer and consequently its performance. For example, if a fracture that intersects a deposition hole is modelled as a planar feature with uniform hydrogeological properties, resaturation will be predicted to occur differently to a case in which the fracture is modelled to as having heterogeneous hydrogeological properties (e.g. flow occurring along effectively 1D channels within the fracture plane).

2. The new Q_{eq} terms calculated by SKB to account for spalling should be checked by reviewing the report on **mass transfer between waste canister and water seeping in rock fractures** (TR-10-42).

3. The way in which the q_{zone} flow rates are calculated/post-processed from SKB's DFN calculations should reviewed for use in the probabilistic corrosion calculations.

4. Additional calculations should be undertaken to confirm that the lowest groundwater salinities that could plausibly be attained (apparently equivalent to around twice the safety function indicator of total ionic strength of cations >4 mM) will not result in a significantly enhanced likelihood of buffer erosion.

5. Data from the DFN model is used in almost all EBS modelling activities, from buffer resaturation to corrosion. The way in which data from the DFN model has been used or post-processed to determine or inform choices of parameters is not always clear. Furthermore it is not apparent that conservatisms and uncertainties that have been investigated from a 'groundwater flow perspective' in the DFN modelling are appropriate conservatisms and uncertainties from the perspective of the various EBS

modelling activities. The way in which uncertainties in the various modelling activities are related should be analysed and SKB's DFN reports should be reviewed in this context.

3.5. Modelling Chemical Alteration of Buffer and Backfill

1. The main SR-Site assessment should include an improved summary of the results of buffer and backfill modelling presented in the report on **aspects of the geochemical evolution of the near-field** (TR-10-59) Section 10.3.10 of the main report of SR-Site (TR-11-01) is entitled "Buffer and backfill chemical evolution", but does not cover the backfill explicitly.
2. The treatment of reaction kinetics in the modelling of buffer and backfill alteration (as described in TR-10-59) needs to be clarified. It appears that kinetics were not modelled, but this is unclear from report TR-10-59. Uncertainties associated with kinetics (rate laws, data, surface areas etc) should be evaluated and discussed.
3. Further discussions of buffer and backfill alteration processes that have not modelled and justifications for their exclusion should be provided. It should be explained why exclusion of processes are insignificant to the conclusions reached (if indeed these processes are insignificant). For example, surface protonation of montmorillonite cannot be modelled by TOUGHREACT, but does exclusion of this process make any difference to the conclusions?
4. Further evidence should be supplied for the assumed insignificance of quantitatively small mineralogical changes, such as the redistribution of carbonate minerals in buffer made from Deponit CA-N bentonite.
5. Inconsistencies between model inputs in TR-10-59 and information in buffer and backfill production reports (TR-10-15 and TR-10-16 resepectively) should be rectified and / or their significance explained. For example, Deponit CA-N bentonite is stated to contain pyrite in TR-10-59, but TR-10-16 states that this mineral is absent.

3.6. Modelling Cement-Bentonite Interactions

1. Additional models should be undertaken to verify previous models of cement-bentonite interactions presented in reports on **evaluation of low-pH cement degradation** (TR-10-62) and **quantitative modelling of cement degradation processes (**TR-10-25). This verification should focus particularly on the sensitivity of these models to the kinetic rates that are assumed and the grid sizes employed. This additional work should include a thorough review of the thermodynamic data that have been used in these models.

4. Review of EBS Modelling in SR-Site

4.1. EBS Safety Functions and Safety Function Indicators

The assessment presented in the **main report of the SR-Site project** (TR-11-01) specifies safety functions that the repository system should fulfil. The overall safety functions are “containment” and “retardation”, which will be achieved if several “lower level” safety functions are fulfilled for the canister, the buffer, the deposition tunnel backfill and the host rock. The reviewers find this approach to be logical and readily defensible. The present review focusses on understanding how SKB has used coupled THMC models of the EBS to support their conclusion that the safety functions of the canister, buffer and backfill will be achieved.

Every safety function has an associated safety function indicator, which is a particular property of a repository component that can be observed or calculated. To judge whether a safety function indicator will be fulfilled, observed or calculated values of the indicator are compared with a safety function indicator criterion. If a safety function indicator fulfils the criterion, then the safety function in question will be fulfilled. The THMC modelling of EBS components covered by the present review is relevant to understanding the safety functions, safety function indicators and safety function indicator criteria Table 2.

Table 2 Summary of safety functions, safety function indicators and safety function indicator criteria within the scope of the present review (designations of safety function, Can1, Buff1 etc are taken from TR-11-01)

Barrier Component	Safety Function	Safety Function Indicator	Safety Function Indicator Criterion
Canister	*Can1*: Provide corrosion barrier.	Copper thickness	>0
Buffer	*Buff1*: Limit advective transport	• Hydraulic conductivity • Swelling pressure	• < 10^{-12} m/s • > 1 MPa
	Buff2: Reduce microbial activity	Density	High
	Buff4: Resist transformation	Temperature	< 100°C
	Buff5: Prevent canister sinking	Swelling pressure	> 0.2 MPa
	Buff6: Limit pressure on canister and rock	• Swelling pressure • Temperature	• < 15 MPa • > −4°C
Deposition Tunnel Backfill	*BF1:* Counteract buffer expansion	Density	High

The safety function criteria corresponding to *Buff2 (*Reduce microbial activity) and *BF1* (Counteract buffer expansion) are each expressed qualitatively; the criteria are stated to be that the density of the buffer should be "High". Without further explanation, these qualitative criteria cannot be judged; what is the meaning of "high". It is unclear why a quantitative criterion cannot be given for these safety functions. Page 243, para 3 of the **main report of the SR-Site project** (TR-11-01) implies that "The repository system will evolve continuously and in many respects there will be no sharp distinction between acceptable performance and a failed system on a sub-system level or regarding detailed barrier features". However, the fact that buffer properties will change gradually does not prevent a density at which no microbial activity will occur from being specified. Similarly, it would be possible to specify a density at which there is no potential for canister sinking. Such criteria will be conservative, because the corresponding safety functions on their own do not determine whether or not the "higher level" safety functions will be achieved. However, it is not clear why such conservatism in these cases is avoided, while in others (e.g. numerical limits on hydraulic properties corresponding to *Buff1*: "Limit advective transport").

According to the discussion in Section 8.3.2 of TR-11-01, the following safety functions of the buffer depend at least partly upon the premise that the buffer will be homogeneous:

Buff1: Limit advective transport;

Buff2: Reduce microbial activity;

Buff4: Resist transformation; and

Buff6: Limit pressure on canister and rock.

Page 254, para 17 of TR-11-01 states that the safety function indicator criterion for *Buff1*, namely that the hydraulic conductivity will be < 10^{-12} m/s, will be fulfilled provided that the swelling pressure, $\sigma s > 1$ MPa. It is argued on page 67, para 6 of the **buffer, backfill and closure process report** (TR-10-47) that1 MPa is also high enough to efficiently fill irregularities on the rock surface in a deposition hole. Hence, until resaturation has proceeded sufficiently for this swelling pressure to be attained, it is possible that irregularities in the walls of the deposition hole will not be filled.

The safety function *Buff2* is stated on page 255, para 3 of the **main report of the SR-Site project** (TR-11-01) to depend upon the density of the buffer. Higher densities favour suppression of microbial activity. No quantitative safety function indicator criterion is given because, it is stated, a number of factors number of factors will govern whether or not any microbial activity is detrimental with respect to the safety functions of the EBS. However, according to this section of TR-11-1, additional microbes, other than those present initially in the buffer material, will be prevented from entering the buffer even at densities much less than the reference density of 1,950–2,050 kg/m^3. However, these assertions appear to depend upon the buffer being homogeneously saturated. Is it possible that a microbial activity in less saturated parts of a partially saturated buffer, where swelling pressures would be relatively low, could be significant with respect to safety functions?

The degree to which the buffer is water saturated will influence its ability to conduct heat and therefore its temperature. Therefore, the potential for chemical alteration of the buffer material is expected to be influenced by the degree of buffer saturation. Consequently, the extent to which the safety function *Buff4* is fulfilled will depend upon the extent to which the buffer has resaturated. Any inhomogeneous resaturation will therefore have implications for buffer alteration.

In the case of the safety indicator *Buff6*, freezing of the buffer is stated to be prevented if temperature remains > -4 °C. However, this criterion is based on the assumption that the buffer is water saturated and has a swelling pressure >1950 kg/m^3. If the buffer does resaturates heterogeneously prior to the next period of glaciation so that a lower swelling pressure is achieved, at least locally within the buffer, then presumably the chances of the buffer freezing will be enhanced.

4.2. Treatment of EBS Evolution in Scenarios

4.2.1. Approach to Scenario Development

In SR-Site, the general approach to scenario development was “top down” in that it initially focussed on the high level safety functions ‘containment’ and ‘retardation’ and subsequently on the other safety functions that impact upon these high level safety functions. A main scenario was specified, based on a reference evolution of the Forsmark site. Subsequently a number of alternative scenarios were identified, each of which corresponds to the loss of one or more safety functions. This approach is considered to be appropriate and consistent with practice adopted in other radioactive waste disposal programmes throughout the world.

Subsequent sub-sections focus on the treatment of the EBS in these evolution scenarios.

4.2.2. Initial State

The initial state is defined on page 19, para 4 of volume 1 of **main report of the SR-Site project** (TR-11-01) as “… the state at the time of deposition/installation for the engineered barrier system and the natural, undisturbed state at the time of beginning of excavation of the repository for the geosphere and the biosphere”. According to this definition, at the time when the engineered components are in their initial states, the surrounding geosphere is not at its initial state.

It is noted in the 3rd bullet point of page 318 of TR-11-01 that “There is a large uncertainty in the detailed salinity distribution around the repository. However, the salinity will not become so high or so low as to affect the performance of the repository during this [the excavation / operational] period or when considering its future evolution”. However, it is unclear that this statement is justified given the coupling between groundwater fluxes, chemistry and buffer / backfill performance. Figure 10-37 indicates that some portions of the rock mass will contain water with 1000 mg/l TDS, while page 358, para 1, line 7 states that “Towards the end of the modelled period 25% of the groundwaters in the repository volume have less than 3 g/L of dissolved salts at repository depth, whereas all the groundwaters had salinities above 6 g/L at the start of the simulation, that is, at repository closure”. That is, some of the water could have a salinity of less than c. 50 mM and possibly less than c.15 mM. Furthermore, there is an implication that at some locations the salinity could vary between c. 100 mM and c. 15 mM as a result of the excavation-related disturbance. While all these salinities appear to be above the minimum level required to prevent colloid formation from buffer materials, it is possible that at the lowest salinities the water may be close to the safety function criterion that cation concentrations should be <4 mM. Some additional discussion of this possibility would be helpful.

The initial state of the emplaced waste is defined for the time when a waste canister has been emplaced in a deposition hole and then sealed with buffer and backfill (page 143, para 4, **main report of the SR-Site project** (TR-11-01)). However, this initial state will not be identical for all deposition holes. There is little discussion of this fact and its significance, although it is stated that consideration will be given to "the common evolution that all deposition holes will go through, taking spatial variability into account" (page 143, para 4, TR-11-01). Some clarification of the meaning of "common evolution" would be helpful.

Page 143, para 10 in TR-11-01 states that the engineered barriers should be adapted to the chemical conditions at the site. That is "The groundwater composition in rock volumes selected for deposition holes should, prior to excavation, fulfil the SR-Can function indicator criteria regarding chemically favourable conditions". However, for assessment purposes the initial condition of the deposition holes is specified to be the conditions at the time of sealing. The reader is caused to wonder whether the function indicator criteria will also be met at this time.

Page 112, para 4 of TR-11-01 states that the current mean temperature at 500 m depth is 11.6°C, based on measurements in 8 boreholes. However, no indication of the variation of temperature, if any, is given. Additionally, paras 2 and 3 on this page also indicate that there is considerable variability in thermal properties between the dominant rock type (medium-grained metagranite) and certain subordinate rock types, such as amphibolite. Presumably, therefore, there will be variations in initial temperature between different canister deposition holes. It would be valuable to indicate this variation.

Page 187 of TR-11-01 discusses the initial state of the buffer and presents evidence that the design premise requiring a minimum swelling pressure of 2MPa will be fulfilled. Although cation exchange is not likely to call this conclusion into question, it would be helpful to discuss the possibility that this process may occur and its potential impact. Figure 5-14 shows only variations in the swelling pressure of MX-80 and Deponit CA-N bentonites as functions of the ionic strengths of coexisting Na-Cl and $CaCl_2$ solutions respectively.

4.2.3. Main Scenario

The reference evolution and the main scenario based upon it are described in Sections 10 and 12 respectively of the **main report of the SR-Site project** (TR-11-01). The main scenario is based on two cases of the reference evolution:

1. A base case in which the external conditions during the first 120,000 year glacial cycle are assumed to be similar to those experienced during the most recent cycle, the Weichselian. Thereafter, seven repetitions of that cycle are assumed to cover the entire 1,000,000 year assessment period.

2. A global warming variant in which the future climate and hence external conditions are assumed to be substantially influenced by human-induced greenhouse gas emissions during the first 120,000 year glacial cycle. This analysis is related to that of the base case.

During the operational phase excavation/operational phase, backfill and buffer will evolve chemically due to the onset of resaturation and the consequent chemical reactions that may occur, and the chemical disturbance to the natural conditions caused by the presence of the repository.

During the operational phase the already installed buffer, backfill and plugs may be affected by the groundwater flow seeping into the open repository. To ensure that safety functions are maintained it is stated on page 323, Section 10.2.4 that:

1. A well-performing plug at the end of a deposition tunnel is needed to ensure that the safety functions related to buffer and backfill density, swelling pressure and hydraulic conductivity are upheld.

2. Homogenisation of buffer and backfill is crucial to fulfil the safety functions related to buffer and backfill density.

It is noted that the reference bottom plate in each deposition hole consists of a low pH-cement concrete slab, and a lower and upper copper plate. The only purpose of the bottom plate is to facilitate the installation of the canister and the buffer. Following buffer installation no more performance is expected from the bottom plate.

In SR-Site geochemical effects are evaluated by using separate specifications for the different climatic domains (page 510, last line in the **main report of the SR-Site project** (TR-11-01).

Page 359. Para 5, line 1 of the **main report of the SR-Site project** (TR-11-01) it is stated that “It may be concluded from these modelling results that for the whole temperate period following repository closure cation charge concentrations at repository depth at Forsmark will, *in general*, remain higher than 4 mM”. What is the meaning of “in general”? This term implies a possibility that at some locations that criterion of 4 mM cations will not be achieved. Indeed, the last sentence of the same paragraph states that nearly one percent of the deposition holes may actually experience “dilute conditions” during the first ten thousand years.

4.2.4. Variant Scenarios / Alternative Evolution

In the SR-Site assessment (**main report of the SR-Site project** (TR-11-01)), scenarios that describe different evolutions to the reference scenario are termed “additional scenarios”. These scenarios are specified according to the factors that cause loss of containment. There are thus:

Three scenarios for waste canister failure, each one corresponding to a failure mode:

- corrosion;
- isostatic pressure; and
- shear movement.

Three scenarios for failed states of the buffer:

- advective;
- frozen; and
- transformed

The canister scenarios are systematically combined with the buffer scenarios. Only scenarios in which a canister fails by corrosion and/or in which the buffer fails are within the scope of this review.

The “additional scenarios” are classified into “less probable” and “residual” scenarios. It is stated (e.g. page 32, para 7 of the **main report of the SR-Site project**, TR-11-01) that “In the former case, the likelihood of the scenario is normally pessimistically set to one”. In contrast the residual scenarios describe additional issues in SSM’s Regulations and General Guidance and are specified to obtain a deeper understanding of barrier functions. However, the precise distinction between the “less probable” and “residual” scenarios is poorly explained. These latter scenarios are defined to be “any other scenarios that are, for any reason, considered necessary in order to obtain an adequate set of scenarios” (e.g. page 32, last para TR-11-01). The “residual scenarios” are further stated to be “hypothetical, residual scenarios to illustrate barrier functions” (8th bullet point on page 33 of TR-11-01). However, all the “additional scenarios” are hypothetical in the strict sense of the word; it is not expected that any of them will actually occur.

4.2.5. Summary of Scenarios Reviewed

In summary, the following scenarios are within the scope of the present review:

- A main scenario, corresponding to the reference evolution.
- A buffer advection scenario exploring the routes to and quantitative extent of advective conditions in the deposition hole.
- A buffer freezing scenario exploring the routes to buffer freezing.
- A buffer transformation scenario exploring the routes to buffer transformation.
- A scenario exploring the routes to and quantitative extent of canister failures due to corrosion.
- Hypothetical, residual scenarios to illustrate barrier functions.

4.3. Conceptual Models of EBS Evolution

4.3.1. Conceptualisation of Hydrogeological Processes

Flow Pathways

Groundwater flow will be along fractures. However, the nature of the fractures that may intersect the deposition holes and their significance should be explained more clearly. According to the Extended Full Perimeter Intersection Criterion (EFPC), large fractures are not allowed to intersect deposition holes (e.g. page 22, para 4 and page 152, para 6, 7, 8 of the **main report of the SR-Site project** (TR-11-01)). However, the precise meaning of “large fractures” is unclear. On page 158, para 2 of TR-11-01 it is stated that the total inflow to a deposition hole must be <0.1 L/min, but it is unclear when and how the actual inflow would be determined. Presumably, this inflow criterion should not be exceeded at any time following excavation of a deposition hole. At the time of excavation the rock mass around the deposition hole is likely to have been dewatered and hence measured inflows could be lower than in the undisturbed rock mass. Presumably, therefore, the inflow is estimated using a DFN model?

Presumably, therefore, a “large fracture” is one that conducts a greater groundwater flux than this value? Additionally, this criterion refers to a single fracture. While fractures are infrequent, presumably there is a small probability that there could be more than one fracture intersecting a deposition hole position. In this case, presumably there is also a possibility that although none of the fractures are classified as “large fractures” they could collectively support as much groundwater flow as a “large fracture”. Some discussion of the likelihood of this situation occurring, and its implications for the assessment would be helpful.

When defining the characteristics of fractures that could intersect the deposition holes without compromising the specified safety function criteria there is an element of circular argument. For example, it is stated on page 150, para 2 of TR-11-01 that “…according to present knowledge the total volume of water flowing into an accepted deposition hole must be less than 150 m^{3}”. It is then stated that for this criterion to be met “Fractures intersecting the deposition holes should have a sufficiently low connected transmissivity (though a specific value cannot be given at this time)”. However, it is also stated that “This condition is fulfilled if the conditions regarding inflow to deposition holes are fulfilled”.

Deposition holes are sited with respect distances to fractures that can “ potentially host large earthquakes” (e.g. 6th bullet of the summary on page 22 of volume 1 the **main report of the SR-Site project** (TR-11-01)). However, it is unclear how it is known that a particular fracture could “host” a large earthquake.

Resaturation

In the **main report of the SR-Site project** (TR-11-01, Section 10.3.8).the discussion of buffer and backfill resaturation commences by stating that the safety functions for the buffer and backfill assume a fully water saturated state. It is then noted that:

“… no performance is needed from the buffer as long as the deposition hole is unsaturated, since no mass-transfer between the canister and the groundwater in the rock can take place in the unsaturated stage. The water saturation process itself has therefore no direct impact on the safety functions of the buffer and backfill.”

A more precise definition of what is meant by “fully water saturated” and “unsaturated” would help the discussion.

The language used suggests that the distinction between “fully water saturated” and “unsaturated” is clear-cut in that a given buffer is assumed either to eventually resaturate completely and uniformly, or to remain unsaturated. It is also stated in TR-11-01 that only the first of these possibilities has any performance relevance, since the presence of a “wet pathway” provides a potential route for corrodants to reach the canister and for radionuclides to leave. However, in buffers that are resaturated from one or two small fractures the distinction is less clear. It is possible that in these cases the buffer would remain in a state of “overall partial saturation” for a long time with regions near the fracture, possibly up to the canister surface, being fully saturated whilst the large amount of bentonite above the canister could remain close to emplacement saturation levels. In this case there would be a connected saturated pathway from canister surface to the fracture but with the buffer still not being fully water saturated. It is not obvious whether such a situation could pose any potential performance issues, but the possibility does not seem to have been addressed by SKB. This may be a consequence of the results of SKB’s modelling, which suggest that the buffer will always completely resaturate. This issue is considered further in the independent modelling investigation in Section 6.

4.3.2. Conceptualisation of Chemical Processes

Buffer and Backfill

The conceptualisation of chemical processes in the buffer is summarized in Section 10.3.10 of the **main report of the SR-Site project** (TR-11-01). A detailed description is given in a report on aspects of the **geochemical evolution of the near-field** (TR-10-59), which is referenced in Section 10.3.10.

Section 10.3.10 of TR-11-01 is entitled “Buffer and backfill chemical evolution”, but does not explicitly discuss the backfill. It would be helpful for the section to state clearly what differences, if any, there are between the chemical evolution of the buffer and the backfill. Alternatively, if these materials will behave similarly, then a clear statement to this effect should be made.

This section of TR-11-01 states that the buffer evolves chemically as a consequence of:

1. thermal effects due to heat production by the waste;
2. water saturation of the bentonite;
3. interaction between the water-saturated bentonite and the local groundwater

In the absence of any discussion of the backfill in this section the reader might well assume that these processes would also affect evolution of the backfill. However, from the detailed discussion in TR-10-59 it appears that in fact only the second and third of these processes are important in the backfill.

After deposition, heat generation from the waste canister produces a thermal gradient across the buffer. Simultaneously a hydraulic gradient will be caused by suction in the unsaturated bentonite blocks and the hydrostatic pressure in the surrounding rock. The solute transport that occurs during the period of heating and water saturation is discussed in TR-11-01on page 398, para 8, which states that in the buffer solutes tend to be transported by advection prior to full water saturation and by diffusion thereafter. Since the saturation rate depends partly upon the water flux through fractures in the host rock, the time of the transition between advection-dominated and diffusion-dominated solute transport also depends upon the water flux in the fractures. However, para 8 on page 398 of TR-11-01 is somewhat unclear about the details of this transition. The first sentence of the paragraph states that advection is the main transport mechanism at periods of up to 2000 years, but the third sentence mentions that if groundwater fluxes are low, then diffusion will dominate after 1000 years.

The absence of a discussion about the backfill in Section 10.3.10 of TR-11-01 will cause readers to assume that similarly there will be a transition from advection-dominated transport to diffusion-dominated transport in the backfill. However, as stated in para 7 of page 23 of the report on **geochemical evolution of the near-field** (TR-10-59), throughout the water-saturated period transport in the backfill is considered to be dominated by advection.

Certain accessory minerals present initially in the buffer are considered to redistribute during the thermal phase owing to their temperature-dependent solublities. These minerals are stated to be anhydrite and amorphous silica in the case of MX-80 bentonite and anhydrite, amorphous silica, calcite and dolomite in the case of Ibeco RWC bentonite. The mentioned minerals are not entirely consistent with the mineralogies that are given in **buffer production report** (TR-10-15). This latter document states that the MX-80 contains gypsum, whereas Ibeco RWC contains anhydrite; Section 10.3.10 of the **main report of the SR-Site project** (TR-11-01) considers only anhydrite. While this is not a serious problem, since the behaviour of gypsum and anhydrite will be similar, these minerals will nevertheless behave slightly differently. More precision and consistency in the discussion would be helpful. Additionally, the text on page 392, para 4 creates the impression that there are no carbonate minerals in the MX-80 bentonite, whereas Table 3-2 in TR-10-15 states that MX-80 may contain between 0 and 1 wt% calcite and siderite.

During the thermal phase, carbonate minerals (if present) and anhydrite / gypsum are thought to precipitate near to the canister and to dissolve further away, owing to the inverse temperature dependence of the solubilities of these minerals. In contrast, the solubility of silica increases with increasing temperature, so that silica dissolves close to the canister, but is precipitated further away.

The extent and nature (spatial distributions and kinds of minerals) of the mineral transformations that occur during the heating and resaturation periods are considered to depend upon the flux of water from the host rock into a deposition hole. A situation in which the groundwater flux is sufficiently great to prevent chemical reactions in the buffer from affecting the host rock is distinguished from one in which the flux is sufficiently slow that solutes from the buffer may diffuse into the host rock and there influence chemical reactions.

It is stated in Section 10.3.10 of the **main report of the SR-Site project** (TR-11-01) (page 397 para 7) that "As long as the maximum temperature is below 100°C and the pH of the water in the rock is below 11 the montmorillonite in the buffer is assumed to stable for the timescale for assessment of the repository (1,000,000 years)". This statement appears to cover all the possible mechanisms by which the smectite may transform, including cation exchange:

- congruent dissolution,
- reduction/oxidation of iron in the mineral structure,
- atomic substitutions in the mineral structure,
- octahedral layer charge elimination by small cations,
- replacement of charge compensating cations in the interlayer.

However, in Section 10.3.10 of TR-11-01 the only reaction of smectite that is discussed in detail is exchange of Na and Ca by K, leading to illitization. There is no discussion of the other possible mechanism, including other cation exchange reactions, notably exchange of Na for Ca. This is a deficiency of this section and should be covered explicitly. Appropriate cross-references to other sections of the report that cover these topics should also be given.

Following the end of resaturation the long-term evolution of porewater chemistry in the buffer will depend upon the flux of groundwater in the adjacent host rock. Two situations are considered in Section 10.3.10 of TR-11-01:

1. Groundwater fluxes are sufficiently low that the final composition of the bentonite porewater differs from the Forsmark groundwater. Diffusion of porewater and solutes from the buffer into fractures within the rock has the potential to modify the surrounding groundwater composition.

2. Groundwater fluxes are sufficiently high that the groundwater composition is almost invariant and solute concentration gradients from the rock towards the buffer are maintained. Therefore, the porewater in the bentonite

evolves to a composition that is similar to that of the Forsmark groundwater.

Section 10.3.10 of the **main report of the SR-Site project** (TR-11-01) also mentions the possible effects of:

1. groundwater salinity on water vapour pressure and hence upon resaturation rate; and

2. cementation of the buffer due to the redistribution of minerals, especially in the thermal phase.

It is concluded in both cases that these processes will have no detrimental effect on buffer performance. This conclusion is reasonable in the case of the groundwater salinity, since very high groundwater salinities (> marine water) are not likely to occur at Forsmark. However, little real evidence is provided in this section that cementation will be insignificant. The only argument offered is that the spatial redistribution of minerals will be limited and hence the effects of cementation will be limited too. Further discussion of this topic should be provided and appropriate references to other relevant sections of the report should be given.

Line 7 of para 10 on page 397 of TR-11-01 states that “There are two main concerns about the effects of cementation on the bentonite buffer; one is an increase in hydraulic conductivity, and the other is an increase of shear strength. This is discussed further in the **buffer, backfill and closure process report** [TR-10-47]”. Since these concerns are important and relevant to buffer performance, readers will expect to see some discussion and justification for the eventual conclusion that the process cementation will not have significantly detrimental effects. It is insufficient simply to reference report TR-10-47. In any case, readers are caused to doubt the statement that cementation is unimportant by the comment in para 1 of page 398 of TR-11-01 that “It is evident that an increased temperature will have an effect on the mechanical properties of the bentonite. The reason behind this is still unknown”. Surely, one potential reason is that increased temperature leads to mineral transformations in the buffer that in turn affect the mechanical properties?

Geosphere Interface

The deep groundwater conditions at Forsmark are summarised in Section 4.8 of the **main report of the SR-Site project** (TR-11-01) and described in detail in a report on **hydrochemical evolution of the Forsmark site** (TR-10-58).

In these reports, the groundwater is interpreted to have chemical characteristics that are the result of complex mixing processes driven by the input of different recharge waters during the history of the site and is summarized in a report on. The water components that are believed to have mixed are: (1) dilute glacial melt waters (fresh); (2) Littorina sea waters (slightly saline); (3) long residence time highly saline waters (brines) present in the fractures and the rock matrix; (4) recently infiltrated meteoric water (fresh); and (5) recently infiltrated Baltic Sea marine waters (around 20% of full marine salinity). These last two water types have only affected the shallowest part of the aquifer system, about ≤ 200 m depth. At repository depth (c. 500 m below the surface) the groundwater salinity varies little, TDS ranging from around 5000 mg/l to 6000 mg/l. However, during future glaciations the mechanical, hydraulic and chemical conditions in the host rock will change, particularly due to the site being covered by glaciers.

At greater depths than 100 m pH is interpreted to be buffered by the calcite system, and groundwater is calculated to be in equilibrium with calcite. There is abundant calcite in fractures and no extensive leaching has occurred in response to past glaciation/deglaciation events.

Deeper than c. 20 m the groundwater is interpreted to be reducing. Between 110 and 646 m most of the Eh values in brackish groundwaters are consistent with a control by metastable equilibrium between aqueous Fe(II) and amorphous iron oxyhydroxide with higher solubility than a truly crystalline phase.

This conclusion is supported by mineralogical investigations that have identified the presence of fine-grained amorphous to poorly crystalline phases now evolving towards more crystalline phases. Dissolved sulphide concentrations are systematically low, possibly due to the precipitation of amorphous Fe(II)-monosulphides, linked to the activity of sulphate-reducing bacteria (SRB). At depths greater than 600 m, the dissolved sulphide concentrations increase, which is consistent with the occurrence of SRB and with the active precipitation of Fe(II)-monosulphides. The iron system at these depths seems to be limited by crystalline oxides, mainly hematite.

The explanation of chemical interactions between the geosphere and the buffer and other EBS components is sometimes unclear. For example, in volume 1 of the **main report of the SR-Site project** (TR-11-01) it is stated in the 5th bullet point on page 29 that “Hydrogen produced by the corrosion of steel and iron repository components is expected to either diffuse away or be used in microbial processes”. This section concerns the reference evolution of the rock, but this bullet point actually describes processes in the buffer. If sulphate reduction is involved, the sulphide produced is expected to react with the iron(II) from the corrosion and increased sulphide levels will not occur due to this mechanism”. However, microbial processes will be impaired by the high-density buffer (as expressed by safety function Buff2) and therefore how will hydrogen be used in microbial processes? In any case, how can any sulphide produced in the buffer be expected to react with iron from corrosion, given that the only iron present is the insert located within the copper canister?

Page 65, 4th bullet point in the **main report of the SR-Site project** (TR-11-01) describes the expected change in chemical conditions in the post-operational phase. It is stated that “The chemical conditions in the host rock after excavation and operation of a final repository are expected to have largely returned to natural conditions in a 100 or 1,000 year perspective”. This statement is imprecise. What is the meaning of “largely returned to natural conditions”? Different chemical parameters will return towards their undisturbed states at different rates. For example, redox conditions and pH may return towards their natural states more slowly than groundwater salinity (depending partly upon the rates of groundwater flow). During the operational phase, the hydraulic drawdown in the repository could cause inflow of water from elsewhere with markedly different salinity to the water present initially (e.g. more saline water being drawn into the repository from greater depths). After closure of the repository the head gradients driving such inflow will disappear and hence the groundwater salinity could remain different from the original salinity for a very substantial period of time (density contrasts would probably provide the main driving force for flow in the absence of a topographical head gradient). On the other hand, oxygen-consuming reactions in the rock mass, such as oxidation of Fe(II) in biotite, would cause conditions to start becoming more reducing as soon as the repository has closed. Some discussion of these issues should be given (or a cross-reference to where these topics are discussed).

Presumably “100 *or* 1000 year perspective” actually means “100 *to* 1000 year perspective”.

It is also stated in Page 65, 4th bullet point in the **main report of the SR-Site project** (TR-11-01) that chemical conditions in the buffer will change to some degree during the period of elevated temperatures. The point is made that this period is very short compared to the assessment time frame of a million years. However, the chemical changes in the buffer depend upon the time taken for the buffer to resaturate. If a particular deposition hole is not intersected by conductive fractures, then presumably resaturation can take a very long time indeed. It would be helpful for some discussion of the relationship between timescales of chemical changes in the buffer and timescales of resaturation to be given here (or else a cross-reference provided to a section of the report that discusses this topic).

Canister / Corrosion

The SR-Site report correctly highlights that the concentration of sulphide in groundwater is a key parameter that will influence the rate and extent of copper canister corrosion. Assumptions about sulphide concentrations are described in Section 4.3.5 of the **corrosion report** (TR-10-66). Most of the assumptions that are made here are conservative in so far as they result in sulphide concentrations that will be higher than natural values, giving rise to over-estimated copper corrosion rates. However, the way in which sulphide concentrations for use in corrosion calculations have been selected from the distribution of observed concentrations is not conservative. The reasons for selecting the sulphide concentrations to be used in these calculations are unclear and claimed conservative assumptions are not well justified. Specific limitations of this section are as follows:

It is stated in the first paragraph of Section 4.3.5 that “Under reducing conditions, dissolved Fe(II) is normally present and the maximum sulphide concentrations are regulated by the precipitation of Fe(II) sulphide”. Reaction 4-31 is then given as the reaction by which aqueous sulphide concentrations are buffered:

$$HS^- + Fe^{2+} = FeS(s) + H+$$

However, TR-10-66 does not state the form of the FeS(s). Most likely it would be a poorly crystalline phase, but a variety of forms are possible with varying degrees of crystallinity. Less crystalline forms would buffer aqueous sulphide concentrations at higher values than more crystalline forms. It is therefore important to include some statement about the nature of the sulphide phase.

This reaction depends upon the pH of the water, which controls the speciation of aqueous sulphur. If the solution is slightly acid, then H_2S and not HS^- would dominate. There should be a statement about the likely variability of sulphide speciation over the observed range of groundwater pH and the consequent implications for the aqueous sulphide buffering reaction.

There is also no justification for the assumption of equilibrium conditions when applying reaction 4-31 to constrain aqueous sulphide concentrations.

Under neutral to alkaline conditions (pH > 7) the precipitation of FeS proceeds via a two-step process (Rickard, 1995):

$Fe^{2+} + HS^- = Fe(HS)_2(s)$ followed by

$Fe(HS)_2(s) = FeS(s) + H_2S$

At pH <7, FeS forms by:

$$Fe^{2+} + H_2S = FeS(s) + 2H^+$$

If aqueous sulphide levels are ppm or greater, the rate of sulphide removal from solution by FeS precipitation is 2 orders of magnitude faster at $pH > 7$ than under acid pH (Rickard, 1995).

The second paragraph of Section 4.3.5 gives the equilibrium constant, K, for this reaction 4-31 as being approximately 10^{-3}. However, no justification for this value is given. There are many different values in the literature, several of which differ substantially from this one given in SR-Site. For example, the PHREEQC database phreeqc.dat gives $K = 10^{3.915}$ for the reaction 4-31 when the solid form of FeS is poorly crystalline (FeS(ppt)) and $K = 10^{4.648}$ for the more crystalline mackinawaite.

The exponent of the equilibrium constant given for reaction 4-31 in the second paragraph of TR-10-66, Section 4.3.5 has an incorrect sign. Rather than the stated value of 10^{-3}, the value should be 10^{+3}. The stated ranges of HS- concentration, 10^{-5} to 10^{-4} M, cannot be obtained for the given values of Fe(II) using reaction 4-31 together with the specified pH ranges and Fe(II) concentrations if $K = 10^{+3}$.

The groundwater sulphide concentrations that are given for use in corrosion calculations are not well justified. Paragraph 3 of Section 4.3.5 in TR-10-66 states that measured sulphide concentrations were often below the limit of detection and that values above this limit are likely to reflect sampling-related SO_4 reduction. These findings are consistent with observations reported in published literature concerning other localities (e.g. UK Nirex Ltd, 1997). Subsequently paragraph 5 of Section 4.3.5 then states that sulphide concentrations used in corrosion calculations were selected from measured groundwater concentrations. The implication is that the selected values are artefacts of sampling and causes the reader to wonder why they were chosen. Although reference is made to a report on **sulphide content in the groundwater at Forsmark** (TR-10-39), which justifies the selected sulphide values more thoroughly, for clarity some explanation ought to be included in Section 4.3.5 of the **corrosion report** (TR-10-66).

It is unclear why corrosion calculations for an intact buffer case used a sulphide concentration taken from the 90% percentile of the measured distribution of sulphide concentrations in Forsmark groundwaters. This approach is inconsistent with the **sulphide content in Forsmark groundwater** report (TR-10-39), which states that “There is, however, a probability that for some deposition location in the repository the surrounding groundwaters may have sulphide concentrations as high as 0.12 mmol/L (~4 mg/L)”. That is, TR-10-39 states that natural groundwater potentially could have a sulphide concentration as high as 10^{-4} mol, the highest value given in the distribution. The chosen 90% percentile value is an order of magnitude smaller and therefore not conservative.

Having stated that the 90% percentile value is used in the corrosion calculations, paragraph 6 of Section 4.3.5 then states that “The extreme choice of using the highest measured value is included as an illustration.” It is not clear what this statement means. Does it mean that alternative calculations were undertaken using the maximum value? If so, then what was the justification for carrying out calculations with the 90% percentile value as well?

Paragraph 7 and the subsequent bullet points in Section 4.3.5 concern the selection of sulphide concentrations that were used in corrosion calculations for the case where the buffer was partially eroded. Several steps to the selection process are described, but no justifications are given. It is stated that the highest groundwater sulphide concentration was deleted from the distribution. Why? This is inconsistent with the statement made in the **sulphide content in Forsmark groundwater** report (TR-10-39) that the highest measured value is a possible real groundwater concentration. It is then stated that a point twice as high as this highest value is added to the distribution. Again, why was this done? Why not add a value three times greater, or four times greater, or some other multiple? Finally, the mean value of the resulting distribution of groundwater sulphide concentrations was used. Again, why? The second step (adding a value twice the measured value) is a conservative step, but the third step (selecting the mean value of the resulting distribution) is not conservative.

4.4. Numerical Models of EBS Evolution

4.4.1. Resaturation and Swelling / Homogenisation

Buffer and backfill resaturation and swelling / homogenisation are discussed in the **Main report of the SR-Site project** (TR-11-01, Sections 10.3.8 and 10.3.9). The modelling work underpinning the discussion is that presented in the **THM modelling report** (TR-10-11). Models of resaturation of the backfill and buffer using the Code_Bright THM code are described in Sections 2 and 3 of TR-10-11 respectively (although only the TH capability of the code were used in the predictive modelling). THM modelling of buffer homogenisation is described in Section 5 of TR-10-11. The focus of the discussion here is on the buffer resaturation and homogenisation but some of the comments may also apply to the backfill.

SKB begin their discussion on saturation of the buffer and backfill by stating that the safety functions for the buffer and backfill assume a fully water saturated state. It is then noted that

"... no performance is needed from the buffer as long as the deposition hole is unsaturated, since no mass-transfer between the canister and the groundwater in the rock can take place in the unsaturated stage. The water saturation process itself has therefore no direct impact on the safety functions of the buffer and backfill."

It would help the discussion if a more precise definition of what is meant by "fully water saturated" and "unsaturated".

The language used suggests that the distinction between "fully water saturated" and "unsaturated" is 'black and white' in that a given buffer is assumed either to eventually resaturate or remain unsaturated and that only the first of these possibilities has any performance relevance, since the presence of a 'wet pathway' provides a potential route for corrodants to reach the canister and for radionuclides to leave. However in buffers that are resaturated from one or two small fractures the distinction is less clear. It is possible that in these cases the buffer would remain in a state of 'overall partial saturation' for a long time with regions near the fracture, possibly up to the canister surface, being fully saturated whilst the large amount of bentonite above the canister could remain close to emplacement saturation levels. In this case there would be a connected saturated pathway from canister surface to the fracture but with the buffer still not being fully water saturated. It is not obvious whether such a situation could pose any potential performance issues, but the possibility does not seem to have been addressed by SKB. This is possibly a consequence of the results of SKB's modelling, which suggest that the buffer will always completely resaturate.

The supporting modelling of resaturation of the backfill and buffer is from report TR-10-11 (Sections 2 and 3 respectively), where, models that are implemented with the CODE_BRIGHT THM code are described. The focus of the discussion here is on the buffer resaturation (TR-10-11 / Section 3) but some of the arguments may also apply to the backfill resaturation.

Section 3.4 of TR-10-11 compares the predicted saturation times from three alternative CODE_BRIGHT models of the CRT experiment (one THM model and two TH models) in order to try to gain some understanding of the sensitivity in resaturation time to the degree of homogenisation of the buffer. The comparison is based around the time taken in each of the models for full (99%) saturation to be obtained at each of three representative points across the buffer. It is not really explained why there is a desire to model resaturation with a TH model when a, presumably better, THM model is available.

The THM model that is used in the comparison is described as "A THM simulation (THM CRT) performed for the Canister Retrieval Test (CRT) experiment". TR-10-11 / Section 5 is devoted to development of THM models to the CRT experiment and their ability to reflect the CRT homogenisation data measurements. Several models corresponding to varying underlying parameter values and assumptions are introduced in TR-10-11 / Section 5 and it is not clear which, if any, of these models corresponds to the THM CRT model used in Section 3. Some clarification of the precise details of the THM CRT model are necessary in order to have confidence in the results that are presented.

Better cross-referencing in general in TR-10-11 would greatly aid the reader. As presented it appears that each section is an entirely separate modelling study, each of which could have been expanded upon and been the basis of a report in their own right.

It is noted that in report TR-10-11 there is a tendency to introduce equations without providing any supporting references or any description of the parameters that are included. For example, see TR-10-11 / Page 124-126. Whilst this is fine for the reader that is already familiar with the material it makes the report mostly inaccessible to the non-expert reader, and together with the lack of good cross-referencing, gives the impression that the report was produced in a hurry.

Although the results of the three buffer resaturation models (the two TH models and the THM CRT model) are compared with one another in Section 3 and some nice discussion is presented, at no point are the results of these models actually compared to the measured inflows in the CRT test. Without this piece of additional information it is difficult to derive any confidence that the models that are presented provide any useful predictive capability or that their relative behaviour has any relevance. Presenting the application of the model to the CRT test inflow and saturation data first would better set the context in which the comparison of models is undertaken. As noted above, several THM models are applied to CRT data in Section 5 of TR-10-11, but the focus there is on homogenisation and no comparison with the measured CRT experiment inflow is presented. The only figure showing the predicted saturations from the (1-D) CRT model appears to be TR-10-11, Figure 5-47, where only the model outputs are shown but the experimental data is omitted. This appears odd given that several other measured outputs from the experiment are compared with the model, such as the void ratio and suction data. It is assumed that one of the THM models from this section of the report is the basis for the THM model that is compared with the two TH models in TR-10-11, Section 3. Therefore there is no basis in the report on which to judge the capabilities of the models at reproducing any known experimental resaturation data.

The two TH models are then applied to a first set of modelling cases comprising 6 variations in rock conductivity (low/high), fracture position (none/canister mid-height/tunnel) and fracture transmissivity (low/high). There are only 6 cases as not all possible parameter combination are explored, presumably because rock conductivity is assumed to be correlated with fracture transmissivity, although this is not stated.

A second set of TH modelling cases is also considered in which selected cases from the first set are modified to have either: an extremely high/low rock conductivity; a high rock retention; an altered initial condition; an altered block retention; and an altered buffer permeability. The modelling that is presented is TR-10-11, Section 3 is good and includes a quite thorough discussion of the effects of varying various properties in the TH models. However as noted above the models themselves have not been shown to reproduce measured inflow data and so this discussion can only be considered in the context of discussing sensitivities of the models, rather than variation that might be seen in the real system.

A similar formulation of the hydraulic properties of bentonite to that presented in TR-10-11 was used in Quintessa's QPAC code to predict the saturation profile in one of the mid-height bentonite rings at the end of the CRT experiment (approximately six years after emplacement). The model is broadly similar to those presented by SKB and was included in the THERESA project modelling intercomparison (THERESA, 2008). The saturation curve predicted by QPAC is shown in Figure 1 together with the corresponding measured data from the CRT test. It is clear from the data that after around 5.5 years, the inner-most regions of the bentonite ring were still yet to fully saturate. This partially saturated region has thickness around 20% of the buffer thickness at the sides of the canister. The QPAC model however clearly over-estimates the degree of saturation in this region. The thickness of a bentonite ring (i.e. perpendicular to the long dimension of a canister) is less than the thickness of bentonite above the canister. Hence, it might be expected that similar models of resaturation above the canister would over-predict the degree of saturation there by an even greater amount than the over-prediction in the bentonite next to the canister. For comparison, the measured saturation on the bentonite cylinder at the top of the deposition hole is shown in Figure 2.

The QPAC modelling referred to above is further developed in Section 6.

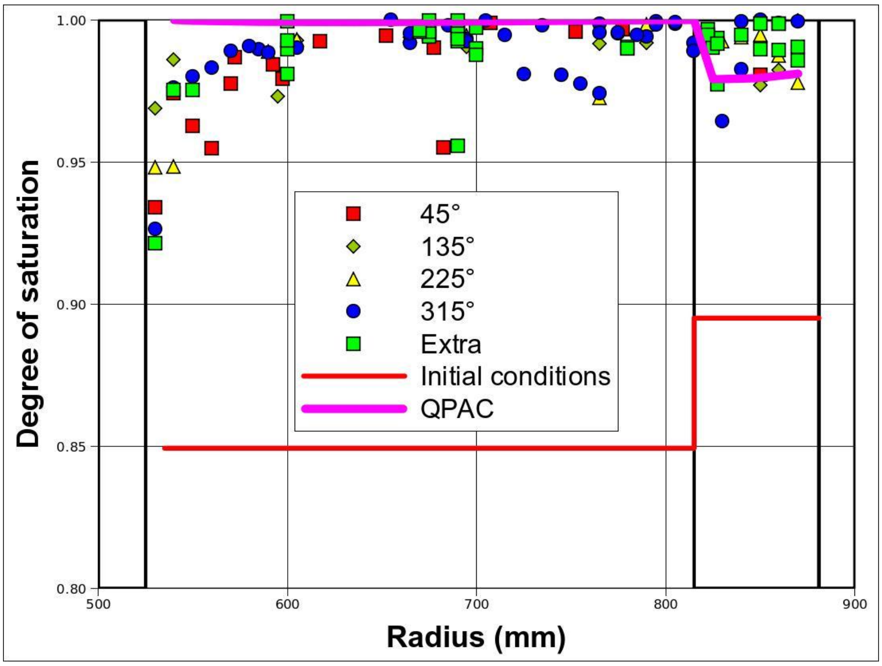

Figure 1 Measured saturation data at the end of the CRT experiment for a buffer location mid-way along the canister. Results of modelling with Quintessa's QPAC code, which includes similar modelling assumptions to those made by SKB, are also shown.

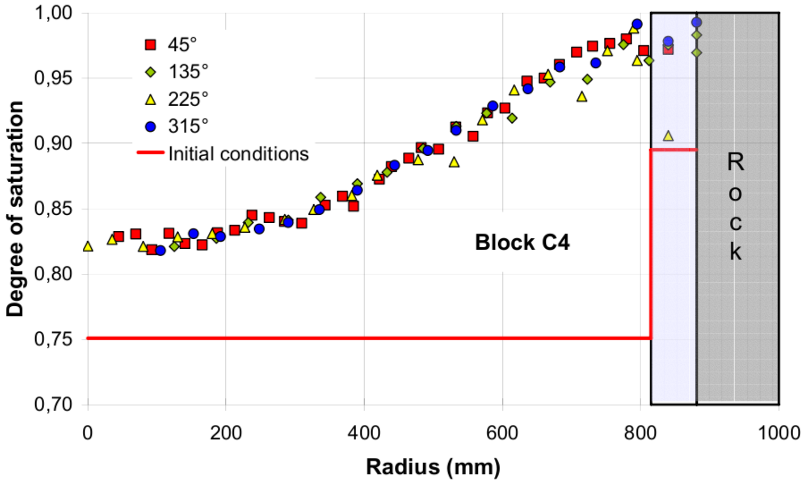

Figure 2 Measured saturation data at the end of the CRT experiment in the bentonite cylinder above the canister (Reproduction of Johannesson 2007, Figure 4-1)

One observation on the models described in TR-10-11 / Section 3 is that they are 'designed to lead to complete resaturation'. That is to say that the suction pressure, which is the driving force for resaturation, leads to in-situ water pressures that are negative whenever the liquid saturation is below 1 and when the liquid saturation approaches 1 the suction pressure tends to zero. . At the emplacement saturation of around 0.85, the suction pressure is approximately 30 MPa in the buffer cylinder blocks and 40 MPa in the buffer ring blocks. The resistance to resaturation is represented by the relative permeability, which is represented in the models as a cubic law on the liquid saturation, hence at emplacement the relative permeability is never especially small. This choice of parameterisation means that the model will always exhibit a tendency to fully resaturate, given sufficiently long, and is a classic formulation used to represent the hydraulic properties of soils and rocks. SKB themselves note that "… phenomenological models developed with typical geomaterials in mind, might have shortcomings when simulating bentonite clay" (TR-10-11 / Section 5.9.3).

Since the main driving force for resaturation in the TH models presented in Section 3 of TR-10-11 is the suction that the bentonite can exert on the water, it might be expected that resaturation should be able to continue in the absence of an externally imposed water pressure, so long at water is present. Figure 3 shows the inflows of water that were measured in the CRT experiment. It is clear that there is a tendency for the inflow curve to 'level off'. Also shown on the graph is the pressure that was applied in the CRT water filter. The data suggests that an increase in the externally imposed pressure was necessary at 700 days in order to allow resaturation to continue, and that resaturation slowed again at around 775 days when the externally applied pressure was removed. This would tend to suggest that the suction pressure alone was insufficient to resaturate the bentonite even when a readily-available supply of water was present, which would appear to contradict the assumptions made in the models. The sensitivity of the model to the externally imposed pressure is compared to the observed sensitivity in the CRT test in Section 6.

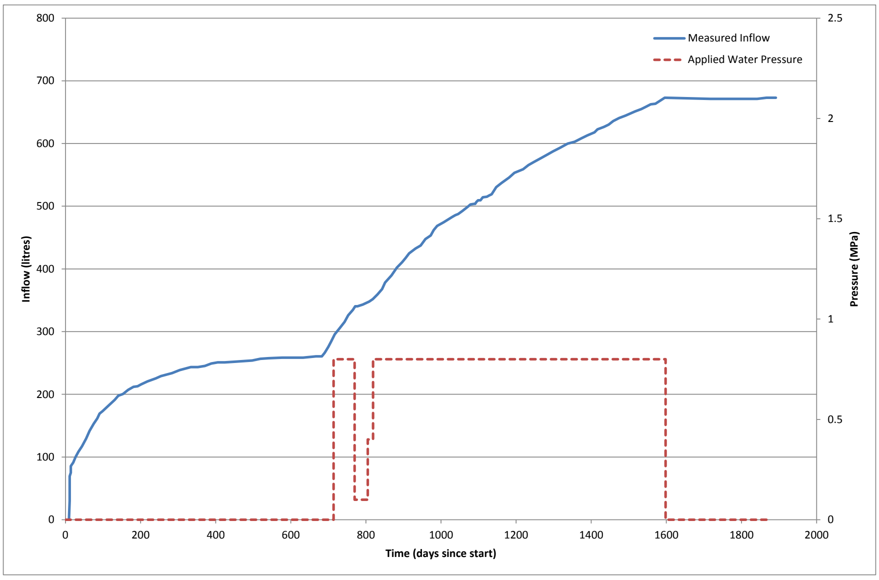

Figure 3 Applied water filter pressure and measured inflows of water in the CRT experiment.

Due to the uniformly-applied boundary conditions on the deposition hole in the CRT test, the maximum distance over which the water in the CRT model had to be 'pulled' is equal to the radius of the deposition hole. The data suggests that the suction pressure that was exerted alone was insufficient to provide this distance of travel. In a deposition hole that is being resaturated from one or two small fractures, water will be less readily available and will have to be pulled over greater distances vertically in the deposition hole, potentially equal to the height of the canister. The

CRT data does not necessarily suggest that this will be possible without an external driving force for the flow, and so it may be possible for hypothetical situations like the one depicted in Figure 4 to arise. Here, the suction pressure (and water pressure at the fracture intersect) has been supposed to be insufficient to draw the water across the entire buffer, or that at least the rate at which water can be pulled into the buffer is slow. An equilibrium, or long-lived situation then arises in which a fully saturated region has developed near the fracture and up to the canister surface, whilst overall the buffer is not resaturated. The consequence is that the swelling pressure in the buffer could remain close to emplacement swelling pressures in some locations, whilst reaching the desired resaturated swelling pressures in others. It is stressed that this is a hypothetical situation and no evidence is present to suggest that it will occur, but equally the evidence from the CRT test would not appear to rule out such a possibility.

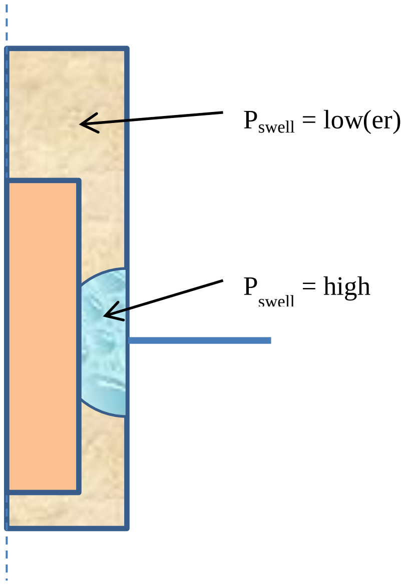

Figure 4 Hypothetical situation that could arise if suction pressure is insufficient to draw water from a small fracture across the entire buffer. A localised fully saturated region connects the fracture to the canister surface while the majority of the buffer remains close to emplacement saturations

As was noted above, SKB have no performance requirements for an unsaturated buffer, but this treats saturation as a ‘black and white’ issue. If the self-limiting behaviour that has been referred to above is genuine, or if behaviour of this type only acts to slow the rate of resaturation, then it is possible that there could be a long time period over which the saturation in the buffer has a pattern similar to that sketched in Figure 4. If this situation were to occur then the following consequences could apply:

- Variations in swelling pressure may exert an uneven load on the canister;
- A localised saturated region may restrict the focus of corrodants transported into the buffer by diffusion from the neighbouring groundwater;
- Microbial activity may not be excluded in some locations; and
- The period of vapour/gas interactions in the buffer would be extended.

SKB do note that the saturation response of the buffer predicted by the TH models have only been compared to those predicted by their THM model "for rapid saturation processes" (TR-10-11, Section 3.6.10). The main reason for this would appear to be that SKB's THM models have only been calibrated against resaturation data from the CRT experiment, where the imposed rates of resaturation were relatively fast (and were from a homogeneous water source along the length of the deposition hole). The type of heterogeneously saturated situation that is hypothesised above would appear to only be possible in situations where there is limited water availability. It is suggested that confirmation of the adequacy of the current TH models **and** THM models in situations where resaturation occurs more slowly is required.

SKB also acknowledge incomplete understanding of how the mechanical behaviour of the bentonite may affect its ability to resaturate under conditions of limited water supply when they state (**THM modelling report** (TR-10-11), page 372) that "The relation between the saturation responses for TH-models and Thermo-Hydro-Mechanical (THM)-models has only been investigated for rapid saturation processes". It is suggested that further investigation of this behaviour may help to understand whether situations like the one sketched in Figure 4 are possible.

One surprising aspect of the results that are presented in Section 3 of TR-10-11 is that the minimum time taken for complete resaturation is around 7 years and that the predicted times for complete resaturation of the buffer from a canister mid-height fracture are only in the range 7-30 years (Figure 5, which is a reproduction of TR-10-11, Figure 10-50). Here, "complete resaturation" is defined as porewater saturation being greater than 0.99 at every location in the model of the buffer. This result appears to be inconsistent with the measured saturations in the uniformly-wetted CRT test after 5.5 years (Section 6). These measurements suggested that not even the bentonite rings up to the canister surface had been fully resaturated in this time. Resaturation over the longer distances to the centres of the bentonite cylinders above the canister would seem unlikely.

It would be useful to hear SKB's comments on this observation and to see the estimated time for resaturation if the TH models were applied to the CRT data.

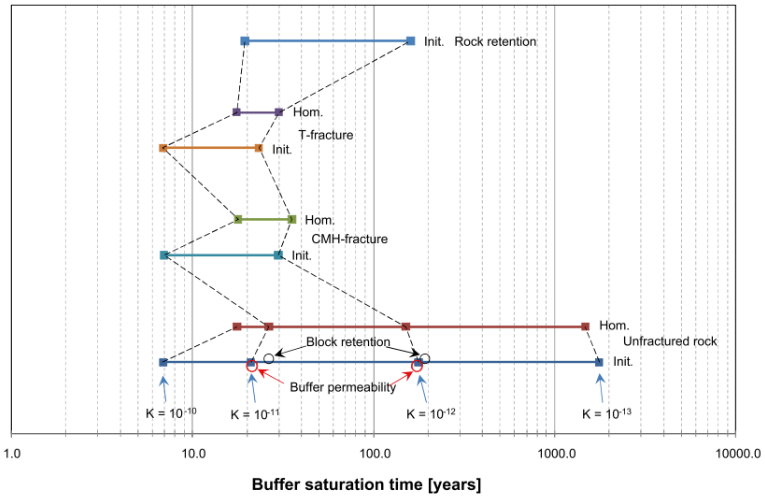

Figure 5 Figure 10-50 from TR-11-01 showing the predicted times for resaturation for various scenarios.

Regarding the tendency of models based on these assumptions to over-estimate the rate of resaturation, in Quintessa's summary of the CRT modelling in the THERESA project (Bond et al., 2009) it is stated that

"... the calculations have demonstrated the difficulty in getting both a good fit to the early-time behaviour... and the longer-term resaturation. Experiments with the 3D model showed that it was not possible to be consistent with both the short-term resaturation behaviour captured by the heavily instrumented Ring 5, and the apparently slower resaturation occurring in the upper cylinders, even when reducing the intrinsic permeability of the cylinders relative to the rings by nearly an order of magnitude.

The 3D calculations tends to over-predict the rate of resaturation and do not fully capture the changing rate of water ingress as water pressures change. It appears that the experiment exhibited a 'sealing' effect at a given water pressure. Once equilibrium had been achieved, increasing the water pressure then caused the system to move to a higher level of saturation and a new equilibrium"

This is consistent with the overall conclusions of the Theresa project (THERESA, 2008), which suggested that in general the current capabilities of models was encouraging, but that

"Hydraulic behaviour, however, appeared to be sensitive to some critical laws and/or parameters: retention curve, relative permeability, gas conductivity, for example. This necessarily might reduce the quantitative predictive power of the formulations."

So it would seem that the "correct" parameterisation of the hydraulic properties of bentonite is not fully understood. Indeed it has been observed in several modelling studies including the CRT that bentonite resaturation does not follow the classic multiphase flow assumptions for static rocks and soils. In particular the availability of pore space within the bentonite for fluid transport is not well understood, and some authors propose that different types of porosity are present (Bradbury and Baeyens, 2002) and that the total porosity will not be available for fluid transport. For this reason it would seem inappropriate to parameterise the hydrogeological properties of the bentonite in terms of a single simple liquid saturation, and in particular the parameterisation of the suction driving force and permeability resistance would not appear to be a correct reflection of the true behaviour in the bentonite.

It is noted that in contrast to the measured inflow data in the CRT test, there is alternative experimental evidence that does not exhibit the type of limiting behaviour discussed above. For example, the measured water content in the FEBEX in-situ experiment (FEBEX, 2012) has been seen to continue to increase over the first nine years of the experiment without any apparent self-sealing. It is noted however that the FEBEX bentonite is a 1:1 Na:Ca bentonite with a lower montmorillonite content than the 4:1 Na:Ca MX80 bentonite and that its hydro-mechanical performance can be expected to be different. For example the measured swelling-suction relationship between the two bentonites is quite different (Cui et al., 2011). For more information see the discussion in Section 6.6. (Ibeco bentonite, which is presented as a potential alternative bentonite in SR-Site has a monovalent :divalent cation ratio of around 1:3.)

The collected experimental evidence would therefore seem to suggest that the THM performance of each bentonite should be evaluated independently for the hydraulic conditions that are likely. In particular, the performance of the MX80 and Ibeco bentonites that are presented as being interchangeable in SR-Site, could in fact be dissimilar. The modelling presented in TR-10-11 is only performed for the MX80 bentonite.

For the reasons listed above, and since it has not been shown that the models presented in the **THM modelling report** (TR-10-11) provide a capability to predict the rates of resaturation that have been observed in experiments such as the CRT test, it is difficult to say with confidence that the predicted rates of resaturation that are presented in TR-10-11 are likely to be truly representative of the possible rates of resaturation in the real EBS environment. This is not to say that the modelling that is presented in TR-11-01 is not good; it does represent the current state of modelling knowledge. Therefore, the question is really whether the current state of modelling knowledge is sufficient to make confidently the type of predictions on resaturation timescales that have been presented.

Issues of interactions between neighbouring deposition holes do not appear to be discussed in the context of resaturation in TR-10-11 or TR-11-01. It is conceivable that in a sequence of deposition holes that are all intersected by the same slow flowing fracture, the first deposition hole in the sequence could locally dewater the fracture and deprive downstream deposition holes of water (if it can exert sufficient suction to distort the local flow field). Thus it may not be sufficient to consider all deposition holes in isolation when computing times to full saturation and the maximum resaturation time for a deposition hole considered in isolation could underestimate that for the ‘last’ deposition hole in the sequence by some margin. Interactions such as this could be a mechanism that could limit the ability of the in-situ hydrostatic conditions to act as a driving force for resaturation in the downstream deposition holes, and possibly lead to the slower resaturation behaviours that have been discussed above. If the period of resaturation is extended in this way, the thermal and chemical evolution of the partially saturated downstream deposition holes could be quite different from those that are upstream.

Independent THM modelling of the resaturation phase is presented in Section 6. There, the tendency for models of the type considered by SKB to fail to reproduce the inflow behaviour that was seen in the CRT experiment is demonstrated and discussed further.

Resaturation and Swelling/Homogenisation – Advised actions

- The TH models of buffer resaturation that are presented in Section 3 of TR-10-11 are not calibrated or compared to the measured inflow data from the CRT test (although other data such as swelling pressure and void ratios are). Without demonstrating that the predictions of the model are consistent with the CRT measurements, and in particular the seeming 'stagnation' of resaturation in the absence of an externally applied pressure seen in the CRT inflow data, it is difficult to be confident in the timescales for resaturation that are presented. The models should be applied to the CRT data to demonstrate that they can reproduce measured rates of buffer resaturation.
- SKB state in TR-11-01 (Page 372) that "The relation between the saturation responses for TH-models and Thermo-Hydro-Mechanical (THM)-models has only been investigated for rapid saturation processes". Further investigation of this behaviour may help to understand whether hypothetical situations are possible in which regions of the buffer can resaturate fully, whilst others remain close to emplacement saturations. In particular, verification of the THM and TH models for slowly resaturating conditions from a single fracture would seem to be required in order to have confidence in the results that are presented.
- SKB should consider the potential for 'heterogeneous saturation' (either permanent or 'long-lived') within the buffer. If it is not considered possible under any combinations of flow and fracture geometry, then arguments should be presented to demonstrate why this is so. If it is considered possible, discussion of the consequences of how it affects the safety functions of the buffer, such as the potential for uneven loading, the possibility of swelling pressures below that needed to supress microbes in some regions and so on.
- Resaturation and homogenisation models are only presented for MX80 bentonite. If bentonite interchangeability is proposed by SKB (e.g. of Ibeco bentonite is a viable alternative), then relevant THM models should be developed for all of the bentonite types that could be considered and calibrated against relevant experimental results, since it is possible that the different hydro-mechanical properties of bentonites with differing monovalent:divalent cation ratios (e.g. Cui et al., 2011) may lead to quite different responses to resaturation . It may be possible to determine general rules specific bentonite behaviour from its monovalent: divalent cation ratio and its montmorillonite content if sufficient experimental data exists. One useful source of experimental information is the FEBEX experiment (FEBEX, 2012), which is closer in composition to the Ibeco bentonite and hence might be expected to exhibit similar hydration behaviour.

Resaturation and Swelling / Homogenisation – Summary of Issues

The modelling performed in TR-10-11 is of a high standard covering a wide range of bentonite THM issues. This review has focussed mainly on sections 3 and 5 (buffer hydration and homogenisation respectively). The following issues have been identified with the report:

- The report TR-10-11 contains a number of spelling mistakes and grammatical errors that suggest that it has not been carefully reviewed. This view would seem to be supported by comments in the **Buffer, backfill**

and closure process report (TR-10-47, November 2010), which post-dates the THM modelling report (TR-10-11, March 2010) and states:

"*The two main reports referred to in the description of the water saturation phase /Börgesson and Hernelind 1999, Börgesson et al. 2006/ are SKB Technical Reports that have not undergone a documented factual- and quality review. However, they are widely referred to by other scientific groups. The revised model of the wetting phase is included in the buffer THM modelling report /- Åkesson et al. 2010a/, which will undergo a documented factual- and quality review."* (Page 65)

"*Buffer homogenisation (both natural during the saturation phase and caused by the sealing of erosion damage) and buffer upwards swelling are reported in old SKB Technical Reports but will be updated and reported in a general buffer THM modelling report that will undergo a documented factual- and quality review /- Åkesson et al. 2010a/.*" (Page 102)

Thus it is not clear whether the THM modelling report TR-10-11 has undergone review. It is possible that a revised version may appear that addresses some of the comments given here.

- Overall TR-10-11 is presented as a collection of independent modelling exercises using different codes and models. There is obviously a lot of overlap and inter-relation between the various sections, for example between the resaturation modelling section and the section on homogenisation. However there is very little cross-referencing within the report to establish these connections. In particular a THM CRT model is used in Section 3 that presumably relates to one of the models presented later in Section 5, but no details of the model are given.
- Due to the 'piecewise' nature of theTR-10-11 report, the reader is left with the impression that 'lessons learned' in one modelling exercise are not being taken advantage of in others. For example the THM models that were developed for the homogenisation study are presumably better models of resaturation than the TH models that were used to make predictions of the time taken to resaturate the buffer and backfill under different assumptions. However, the decision appears to have been made to simulate resaturation as a TH process, with little justification given to why the mechanical component of the model is omitted. This appears strange when similar THM models are presented in the same report (but are only applied to the Canister Retrieval Test data).
- A lot of modelling results are presented in TR-10-11 but there is relatively little discussion of the consequences of the results on the performance of the system. For example, TR-10-11 / Section 5.19 is the conclusion section for the homogenisation modelling. It is less than half a page in length. Key uncertainties in the model are identified, but no discussion is given of the implication of these uncertainties in drawing conclusions on how the real system will evolve, especially under conditions of lower water availability that may be more relevant for in-situ conditions.
- The referencing back to data sources in TR-10-11 is very poor. Model parameter values are introduced with no explanation and the reader is left unsure whether these values arise from measurements, modelling best fits or expert guesses. E.g. TR-10-11 / Table 3-1 gives MX-80 properties used to parameterise the model but no references are given for the data values. In particular, the van Genuchten water retention curve parameters, which are a key control on the rate of resaturation, are simply stated without reference. Many of the data values have subsequently been traced to the

THM modelling buffer, backfill and other system components report (TR-10-44) but this report is not referenced in the THM modelling report TR-10-11, which may be because it post-dates the modelling. It may be the case that the modelling report is the source of the data (with the bentonite mechanical properties for example having been obtained as best fits in the modelling report) but this is not clear.

- Equations and constitutive relationships are introduced in TR-10-11 with no reference to explanatory texts and often without any description of the terms appearing in the equations or their units (e.g. see TR 10 11, page 124). The non-expert reader would most likely find these aspects of the report impenetrable, which detracts from the modelling, which is of a good standard.
- The THM modelling section (TR-10-11 / Section 5) is primarily an application of various models (an analytical model, a Code_Bright model and an Abaqus model) to data measured in the Canister Retrieval Test. The main focus of the section is on modelling performed with Code_Bright, with several modelling variants with different parameters (CRT 1/3/4/6b/9b4/10b…) being compared to the measured data. Different choices of parameterisation provide better fits to different aspects of the CRT dataset. This provides useful information on the sensitivities of the model, but it would have been expected that a best/favoured model would then be identified to define a definitive set of parameters that should be used in subsequent modelling. Results from the Abaqus modelling are presented with little discussion.
- (Following previous point) It would have been expected that if a 'best' THM model had been identified in TR-10-11 it would be applied to a range of likely in-situ conditions, in particular to situations when resaturation occurs from fractures rather than from the idealised CRT hydraulic boundary conditions, which are not representative of the likely in-situ repository conditions.
- Nowhere in TR-10-11 are the results of the TH (Section 3) or THM (Section 5) models directly compared to the measured CRT inflow data. Modelling the CRT experiment is the focus of Section 5, but the main objective is on an investigation of buffer homogenisation rather than resaturation. The only figure showing the predicted saturations from the (1-D) CRT model appears to be TR-10-11 / Figure 5-47, where only the model outputs are shown but the experimental data is omitted. This appears odd given that several other measured outputs from the experiment are compared with the model, such as the void ratio and suction data. It is assumed that one of the THM models from this section of the report is the basis for the 'THM CRT' model that is compared with the two TH models in Section 3. Therefore there is no basis in the report on which to judge the capabilities of the models at reproducing any known experimental resaturation data. Without demonstration of a good fit to the inflow data, which is obviously a key factor in determining the timescales for resaturation, it is difficult to have confidence in the credibility of the TH models that are used to estimate resaturation times under repository conditions.
- Issues of interactions between neighbouring deposition holes do not appear to be discussed in the context of resaturation in TR-11-01. It is conceivable that in a sequence of deposition holes that are all intersected by the same slow flowing fracture, the first deposition hole in the sequence could locally dewater the fracture and deprive downstream deposition holes of water (if it can exert sufficient suction to distort the local flow field). Thus

it may not be sufficient to consider all deposition holes in isolation when computing times to full saturation and the maximum resaturation time for a deposition hole considered in isolation could underestimate that for the 'last' deposition hole in the sequence by some margin. Interactions such as this could be a mechanism that could limit the ability of the in-situ hydrostatic conditions to act as a driving force for resaturation in the downstream deposition holes. If the period of resaturation is extended in this way, the thermal and chemical evolution of the partially saturated downstream deposition holes could be quite different from those that are upstream.

- Models of the rheological behaviour following loss of buffer mass (e.g. after piping erosion prior to full resaturation/homogenisation or after a period of erosion caused by intrusion of dilute glacial meltwaters) are discussed in Section 10.3.9 of TR-11-01. The discussion is based on the modelling presented in Section 6 of TR-10-11. The results of the modelling are interesting and appear plausible. However since the models have not been applied to any experimental datasets it is difficult to be confident in the results beyond the general behaviour that is portrayed. It is suggested that further experiments are performed in this area to develop a useful dataset that can be used to establish confidence that the rates and patterns of 'healing' that are displayed in the models provide a reasonable match to measured data.

4.4.2. Corrosion and Erosion Processes

Copper corrosion processes are summarised in the **main report of the SR-Site project** (TR-11-01) for the operational period (Section 10.2.5) and for the temperate post-closure period (Section 10.3.13). Supporting copper corrosion calculations for the SR-Site safety assessment are given in the **corrosion report** (TR-10-66).

Corrosion Due to Corrodants Initially in the Repository

Some corrodants or corrodant sources are initially present in the repository. These include initially entrapped oxygen, oxygen generated via gamma radiolysis of water, nitric acid from gamma irradiation of moist air and sources of sulphide (e.g. pyrite in the bentonite).

Of the oxygen and radiolysis based processes, the **main report of the SR-Site project** (TR-11-01, Section 10.2.5) lists corrosion due to initially entrapped oxygen as the major corrosion process accounting for up to a 500 µm depth of corrosion arising from the reaction

$$4\,Cu + O_2 \rightarrow 2Cu_2O$$

The 500 µm depth value is stated in the **corrosion report** (TR-10-66, Section 5.2.2) following a simple mass balance calculation (equations 5-5, 5-6) to estimate the total potential amount of reacting oxygen. Such a calculation is appropriate since the amount of initially trapped oxygen that is present is limited and cannot be replenished by the groundwater, except for glacial meltwater intrusion, which is discussed below.

If all of the initially trapped oxygen were to attack the canister surface evenly SKB calculate that the corresponding corrosion depth would be 768 µm and that if the oxygen were assumed to attack only the lid and the top 10% of the canister surface, the depth of corrosion would be at most 5.5 mm.

These results have been verified with a separate spreadsheet calculation: estimates of 758 µm and 5.5 mm were obtained. The minor discrepancy in the first value is most likely due to the fact that the dimensions (height and radius) used for the deposition hole and waste package in the calculation are not stated in the **corrosion report** (TR-10-66). In the verification calculations, values from the **data report** (TR-10-52, p17) were used.

In the **corrosion report** (TR-10-66) mass balance calculations are presented to determine maximal amounts of corrosion due to initially entrapped corrodants / corrodant sources. These calculations appear to use inconsistent datasets to other reports (e.g. tunnel dimensions), and use bentonite porosities that lead to a conservative estimate of the amount of entrapped corrodant. The amounts of corrosion are nevertheless small so this does not impact greatly on the safety case, but inconsistent use of data across the SR-Site reports is not desirable.

Porosity in the mass balance calculations is apparently not treated in the most conservative way:

The calculation (equations 5-5, 5-6) assumes a buffer porosity of 0.4. This is the smallest bentonite porosity given in the data report (TR-10-52), which states the range of buffer porosities to be 0.41-0.46. Moreover, these are the expected porosities from the saturated system. It would seem more appropriate to use the larger emplacement porosities to be consistent and conservative in the estimate.

The calculation assumes that the backfill porosity is the same as the buffer. However the data report (TR-10-52) states that saturated backfill porosities are likely to be in the range 0.44-0.48 (note that there appears to be an error in the data report in the way in which these porosities are quoted – the relationship with density appears wrong (it seems to be inverted)). Assuming the largest porosity value (0.48) would increase the amount of entrapped oxygen in the bentonite pore space by 20% and increase the corrosion depth estimates to 817 µm and 5.9 mm.

The tunnel dimensions given in the calculation have a width and height of 4.2 m and 5.8 m. However the **backfill production report** (TR-10-16, Figure 2-1) gives the tunnel maximum height as 4.8 m. Using this tunnel height, the maximum corrosion depth values are reduced to 632 µm and 4.5 mm respectively.

The 6 m canister spacing that is used in the calculations could not be found in the data report.

On balance, the over-estimation of the air content due to the discrepancy in the tunnel dimensions (compared to the dimensions stated in the **backfill production report**, TR-10-16) out-weigh any discrepancies due to alternative assumptions on the initial bentonite porosities and therefore the amount of air calculated by SKB in equations 5-5, 5-6 is likely to be an over-estimate and hence conservative, assuming that the tunnel dimensions in TR-10-16 are correct. If the tunnel dimensions in the **corrosion report** (TR-10-66) are correct, then the upper bounds that are presented are slightly too low and should possibly be adjusted for the initially emplaced bentonite porosity.

It is correctly stated that these are pessimistic estimates, which ignore the fact that some oxygen will be consumed in reactions in the buffer and backfill and some will diffuse away from the canister. SKB go on to argue that the depth of corrosion due to initially trapped or atmospheric oxygen can be expected to be 500 µm at most when less conservative assumptions are made.

One of the arguments that are given is based on work in (Wersin et al. 1994) that concluded that anoxic conditions would be attained in the repository within t=300 years, from which it is estimated that a corrosion depth of at most 260 µm will be attained if only the top 10% of the canister is affected.

This calculation has been verified: Based on the assumed bentonite effective diffusion coefficient in the buffer ($D_e=1.2\times10^{-10}$ m^2/s) the notional diffusion length for this period is $\sqrt{(D_e\ t)}=1.07$m. SKB use 3 m as a conservative upper bound on this length and assume that all of the oxygen initially trapped in a cylinder with cross-section equal to the deposition hole area and with height 3 m is able to corrode the relevant surface area. The volume of this cylinder is approximately 5% of the volume of the backfill per canister and hence around 5% of the previously calculated maximal corrosion depth of 5.5 mm for the top 10% of the canister would be expected to be a close upper bound. This equates to 275 µm or corrosion, which is close to the value calculated by SKB.

SKB's estimates of corrosion due to gamma radiation have not been reviewed in this initial review phase.

After all of the available oxygen for reaction has been consumed in corrosion or mineral reactions or has migrated away from the canister, the dominant corrosion mechanism that remains is assumed to be corrosion due to sulphide in the groundwater. The availability of sulphide for reactions will depend on its abundance in the groundwater and its ability to migrate to the canister surface. Additionally, sources of sulphide in the buffer and backfill could contribute to the amount of sulphide that is available for corrosion.

The **corrosion report** (TR-10-66, Section 4.1) derives formulae that can be used to compute the rate at which a front of pyrite depletion might sweep across the buffer (away from the canister).

It is not stated explicitly in TR-10-66, Section 4.1 that the analysis that is presented is for a 1-D Cartesian geometry (in the sense that TR-10-66, Equation 4-2 is exact in 1-D Cartesian coordinates but is only an approximation in cylindrical coordinates). A 1-D cylindrical analysis would be more appropriate to the geometry at the sides of the canister; the analysis given is more relevant for the top and bottom.

The **corrosion report** (TR-10-66, Section 5.3.1) states that if all of the pyrite initially present in the buffer were to be converted to sulphide and subsequently corrode the canister, the maximum corrosion depth would be 0.1 and 0.9 mm on the sides of the canister for MX-80 and Ibeco-RWC bentonite respectively. The corresponding depth of corrosion on the lid is calculated to be 0.4 and 2.9 mm respectively, which is well below the 5 cm overall copper thickness. These estimates have not been reviewed in this initial review phase.

The assumption that all of the possible sulphide from pyrite were to become available is conservative. The depletion front model is applied to show that less than 2 cm of pyrite depletion could be expected for both bentonites. With reference values for transport and solubility, corrosion depths up to only 1 µm are expected. With pessimistic transport and solubility assumptions, up to 40 cm of pyrite would be depleted, corresponding to all pyrite to the sides of the canister, with corrosion depths of up to 114 µm.

This calculation could be independently verified although the bounding mass balance calculation above suggests that maximal corrosion depths will be well below the 5 cm copper thickness. Hence reproduction of this calculation is not so vital.

SKB correctly conclude that the amount of corrosion that can be expected due to corrodants or corrodant sources initially present in the buffer and backfill are small compared to the thickness of copper, with the major contribution towards the potential corrosion coming from the initial pyrite inventory in the bentonite, which could lead to corrosion depths of up to 0.4 and 2.9 mm on the side and top of the canister respectively, but which are likely to be over-estimates.

Corrosion Due to Ingress of Corrodants

Having ruled out significant amounts of corrosion from initially entrapped corrodants or corrodant sources, the only conceivable route for additional corrosion is from corrodants entering the buffer system from the host rock. Corrosion due to sulphide in the groundwater and oxygen in the groundwater during periods of glacial melt water intrusion is estimated using SKB’s equivalent flow rate approach. The mathematical treatment in both cases is the same, with only parameter values for O_2 and sulphide (stoichiometric factors and groundwater concentrations) being different. The corrosion reaction that is assumed for sulphide is

$$2\,Cu + HS \;\; + H+ \rightarrow Cu_2S + H_2$$

In the **corrosion report** (TR-10-66, Section 4.2), equivalent flow rate terms (denoted Q_{eq}) are presented for the transport pathways relevant for corrosion. These comprise a pathway from an intersecting fracture through the buffer to the canister surface, and a second pathway in which a region of thermally-induced spalling is represented.

Some of the Q_{eq} terms date from SKB reports that were reviewed as part of the SR-Can submission, but some terms appear only in the more recent reports, such as the report on **mass transfer between waste canisters and water in rock fractures** (TR-10-42). This latter report should be reviewed in detail as a separate task, since it contains details of the mathematical model that SKB use both to model corrosion and also to model radionuclide transport out of the buffer. The same comment applies to both the report on **mechanisms and models of bentonite erosion** (TR-09-35) and the report on **modelling of erosion of bentonite gel by gel/sol flow** (TR-10-64). These two reports are stated as being the basis of the bentonite erosion model that is presented in Section 4.3 of the **corrosion report** (TR-10-66).

The equivalent flow rate approach to mass transport has the attractive feature that once Q_{eq} terms have been derived, the calculations to analyse mass transport are simple (they can be performed in spreadsheets), allowing them to be applied to the range of flow rate data arising from SKB’s DFN calculations. However they do include a number of simplifying assumptions, most notably on the geometry of the pathways that the migrating solutes can take. These assumptions are typically valid at “simple” locations but will become less accurate at more “complicated” locations. For example, a fracture intersecting the buffer at the canister mid-height will see an even canister surface in all directions from the point of ingress and so diffusion will act symmetrically in the buffer and “infinite medium” approximations are likely to be accurate; however solutes entering from a fracture intersecting the buffer near the top of the canister height will exhibit a less symmetrical plume where the approximation introduced by any infinite medium assumptions will be less accurate.

The equivalent flow rate approach is considered to be an efficient method for calculating likely amounts of corrosion for the range of fracture geometries and flows that arise from the DFN calculations. However, the individual Q_{eq} terms that govern the transport should be checked both for analytical correctness and also in terms of the accuracy of their approximation to the range of geometrical arrangements that could arise. It is important that the accuracy of transport formula that arise from these simplifications is understood. Given the role of the transport model in the overall assessment calculations it is necessary that the accuracy is sufficient (in some sense) or that the resulting transport rates can be shown to be conservative. It is noted that assumptions that might be treated as conservative from the point of view of transport of corrodants entering the buffer may not be conservative when applied to radionuclides leaving the buffer.

Since the Q_{eq} approach is only able to provide estimates of the average amount of corrosion, a Buffer Concentration Factor (BCF) is used to represent the focussing of corrosion at locations on the canister surface closest to the fracture (**corrosion report**, TR-10-66, Equation 4-19). The maximum value is taken to be 7, which is derived from a single calculation (SKI, 2006), in which it is assumed that the intersecting fracture with an aperture of 1 mm is located approximately mid-way along the canister height.

The accuracy of this estimate for other fracture configurations has not been demonstrated by SKB. Scoping calculations are presented in Section 5.1 of this report, which investigate the accuracy of the BCF value for other fracture configurations and suggest that a factor of 7 is not always appropriate or conservative.

The **corrosion report** (TR-10-66), Section 5.3.4 specifically states that calculated corrosion rates are over-estimates because "all fractures are assumed to intersect the part of the deposition hole where the canister is located". The scoping calculations that are presented in Section 7.1 suggest that this statement is not true; fractures intersecting at the top of the canister height appear to lead to more focussed corrosion.

In light of the investigation in Section 7.1 it would appear worthwhile to further investigate the range of possible BCF parameters for other geometrical configurations.

The new Q_{eq} term for the thermally induced spalling zone (TR-10-66, Equations 4-8 to 4-11) include the flow rate in the spalling zone as a factor. This is treated as a constant in the analysis, but is likely to vary along the height of the spalling zone away from the intersecting fracture. TR-10-66 states that this (and other) flow rates are "calculated from the output of the hydrogeological DFN model" although details of the 'calculation' (or a reference to the calculations) are not given. The way in which these flow rates are derived will determine whether the Q_{eq} approach is conservative in its approach, but this cannot be assessed from the information that is given in TR-10-66.

SKB concludes that oxygen penetration during glaciation will not be a concern for corrosion (TR-10-66, Section 5.2.3). This conclusion is based partly on an interpretation that the oxygen concentration in the water recharging beneath a glacier will be less than "the theoretical upper limit of 1.5 mM" (page 26, para 6, line 3). Although it may be reasonable to state that penetration of such oxygen-bearing water will not cause unacceptable levels of corrosion it is strictly inaccurate to refer to the concentration of 1.5mM as a "theoretical upper limit". This concentration is only a maximum value for the specific set of pessimistic assumptions that are made. This point should be made clear and it should be explained, briefly why the assumptions are pessimistic. It is inadequate simply to reference Section 12.6.2 of the **main report of the SR-Site project** (TR-11-01) to support the argument that the stated oxygen concentration of 1.5 mM is pessimistic (page 26, para 6, line 7 of TR-10-66). This section of TR-11-01 simply re-states the text given on page 26 of TR-10-66 and references a separate report on **oxygen ingress in the rock at Forsmark during a glacial cycle** (TR-10-57). This cross-referencing is another example of the poor presentation of supporting information that is a feature of the SR-Site documentation. Readers of the **main report of the SR-Site project** (TR-11-01) need to be able to judge whether or not the proposed repository at Forsmark will be safe, based solely upon the arguments presented in this document; they should not need to follow a long trail of documentation to obtain even a basic explanation of a key argument. Furthermore, it is odd that TR-10-66, which is supposed to support the SR-Site safety assessment references the main report of the project to justify its arguments.

The **corrosion report** (TR-10-66, Section 4.3.3) attempts to establish the height of the area that might be exposed on the canister surface due to erosion. The discussion is a little unclear in places as initially a square cross-section hole stretching from the rock wall to the canister surface is discussed where it is stated (TR-10-66, Section 4.3.3, para. 2) that “imagining the geometry growing with a semicircular cross section would only give a factor $\pi/2$ larger volume when the eroded space reaches the canister wall”. However the remainder of the section is then devoted to an analysis based on the semicircular case.

It is correctly stated in **corrosion report** (TR-10-66, Section 4.3.3) that a smaller exposed area would experience a greater rate of corrosion. Arguments are then presented to try to justify why the exposed area is unlikely to remain small. These arguments are based on the assumption of a semicircular geometry which, whilst possible, is not actually known to be the true geometry that will evolve around a point of erosion. It would strengthen the safety case if arguments could be presented, or more mechanistic calculations could be performed, that would either justify, or lead to a better understanding of, the likely erosion geometries that might occur. This would help to determine whether the corrosion areas that are suggested are truly based on conservative assumptions.

Similar to the sensitivity of the amount of copper corrosion to the location of the fracture intersection in the deposition hole (as implied by the calculations in Section 5.1) it is likely that the exposed corrosion area will depend on the location of the fracture. Fractures near the top of the canister will tend to expose areas on the side and lid. However the increased amount of buffer above the canister may allow the bentonite to “heal” more rapidly in that area, resisting the emergence of the erosion zone and confining its influence to the side of the canister. This could result in a smaller exposed corrosion area than is hypothesised in the **corrosion report** (TR-10-66, Section 4.3). The sensitivity of the corrosion area to the location of the fracture should be investigated.

With the assumption of an eroded area with a semi-circular cross-section, the **corrosion report** (TR-10-66, Section 4.3.3) states that the exposed corrosion area will grow rapidly once the canister surface is reached. Whilst it is true that a semicircle with marginally larger radius will have a greatly increased corresponding corrosion area, the rate at which this contact area will appear will be dependent upon the rate of growth of the eroded area. TR-10-66 assumes a “constant growth rate of a semicircle”. The precise meaning of the constant growth rate is not clarified but the nature of the discussion would tend to suggest that the growth rate of the radius of the semicircle is assumed constant (i.e. dr/dt=constant, where r is the radius of the semi-circular cross-section). If there is any buffering of erosion by the presence of bentonite colloids in the eroded hole then it is possible that the rate at which colloids can be removed from the eroded hole could be the erosion rate limiting factor. In this case it would seem that the growth rate of the area of the semicircle is more likely to be the rate that is constant, since the cross-sectional area is proportional to the amount of bentonite colloids that have been removed from the system. For a semi-circular hole, the rate of change of the eroded cross-sectional area is related to the growth rate of the radius by $dA/dt = \pi r\, dr/dt$ and so if the rate of growth of the area is constant it would be the case that $dr/dr \propto 1/r$. Under these assumptions the rate of growth of the radius of the semicircle is therefore decreasing with time. This possibly strengthens arguments that might suggest that the canister will not be reached at all, but weakens the argument that the exposed area would grow quickly if the canister surface was exposed.

A bounding case is described in the **corrosion report** (TR-10-66) based on the "very pessimistic assumption that the erosion stops immediately after it has reached the canister wall". The reasoning for this assumption being considered pessimistic is that it requires an abrupt change in groundwater conditions from dilute to saline to halt the erosion. As noted above there are geometrical arguments that suggest that a slow growth of the exposed area might not be unlikely. Furthermore it is possible that complete erosion to the canister surface might not be achieved in a single glacial period. It may take several periods of glacial meltwater intrusion to fully erode up to the canister surface. In recent work (SSM 2011:12), a hypothetical buffer erosion / corrosion model was studied in which six periods of glaciation were required to erode the buffer up to the canister surface. If this is the case, each period of erosion would be gradual and the chances of a glacial period ending close to the time at which the canister surface is met are increased. In the inter-glacial periods the partially eroded buffer will lead to more rapid corrosion on the canister surface due to the reduced transport distance through the buffer and so overall the rate of erosion will be increased. It is not clear whether corrosion from these repeated glacial cycles are treated in the analysis in TR-10-66 or in the spreadsheet calculation.

The focus of the **corrosion report** (TR-10-66, Section 4.3.3) seems to be on complete erosion up to the canister surface. It is not specifically noted that due to the approximately inverse-proportional dependence of transport distance of corrodants in the buffer on the flux, any reduction in the buffer thickness will lead to an increase in the rate of transport of corrodants to the canister surface. For example, if the buffer thickness is halved by erosion the corrosion rate would be expected to be approximately two times greater than in the case where the full buffer thickness is maintained. Whilst this is perhaps obvious it would be a useful addition to the discussion that is presented. The revised Q_{eq} terms presented in TR-10-66, Section 4.3.2 appear to account for this enhancement in the transport rates but this has not been thoroughly checked.

An upper bound on the corrosion height is derived in the **corrosion report** (TR-10-66, Section 4.3.3) to be 0.7 m. This calculation uses the BCF value of 7 discussed earlier and is calculated by dividing the canister height by 7. However, the derivation of the BCF value of 7 in SKI (2006) is based on the relative corrosion rate experienced over the whole canister surface (i.e. including the lid and the bottom of the canister). Therefore it is not quite correct to apply a scaling of 1/7 on just the canister height. The maximum height for corrosion should be $h_{corr}=(r_{can}+h_{can})/7$, which is larger than the stated upper bound. Again it is noted that BCF values up to around 21 have been calculated for alternative locations of the fracture (see Section 5.1 of this review), which suggests that this upper bound may be more like $h_{corr}=(r_{can}+h_{can})/21$ for other fracture configurations.

The probabilistic corrosion calculations with erosion make use of an 'erosion time'calculation described in the report on **mechanisms and models of bentonite erosion** (TR-09-35) and the report on **modelling of erosion of bentonite gel by**

gel/sol flow (TR-01-64). These should be reviewed. From the summary given in the **corrosion report** (TR-10-66, Section 4.3.1) it would appear that this timescale is only determined by the fracture aperture and flow rate and is not dependent on the fracture location.

The estimates of the amount of corrosion that could arise as a consequence of the anoxic corrosion process presented in section 5.4 of TR-10-66 have not been reviewed in this initial review phase.

Canister / Corrosion – Advised actions

The discussion in the preceding sections and the supporting investigative calculations in Section 5.1 raise questions over the mathematical treatment of corrosion/erosion. A more thorough review of report the **corrosion report** (TR-10-66) and its underlying references should be undertaken to assess the potential magnitude of differences in calculated probabilities of canisters experiencing corrosion over the full depth of the copper casing in the 1,000,000 y assessment period.

4.4.3. Chemical Alteration of Buffer and Backfill

Outputs from numerical models of mass transport and chemical processes in the buffer and backfill are summarized in Section 10.3.10 of the **main report of the SR-Site project** (TR-11-01). The numerical modelling is described in detail in a report on aspects of the **geochemical evolution of the near-field** (TR-10-59). The computer software packages used to implement the models were:

1. TOUGHREACT (Xu et al., 2008), which was employed to produce 1D radial-symmetric simulations of the buffer that represented variably water-saturated multi-phase flow under non-isothermal conditions; and

2. PHAST (Parkhurst et al., 2004), which was employed to produce 3D simulations of the interactions between groundwater and fully water-saturated bentonite.

It is stated on page 9, para 11 that TOUGHREACT does not account for changes in certain physical properties of the buffer (pore deformation due to mechanical stress or swelling; fluid pressure changes due to porosity changes; and heat effects from chemical reactions, such as changes in thermo-physical properties of fluids (viscosity, surface tension and density). However, there is no discussion or exploration of the possible significance of these limitations.

On page 11, para 12, it is noted that PHAST can take as input only a single diffusion coefficient for all the materials that are represented in a model. A value of 2.8×10^{-10} m^2/s was chosen for the diffusivity in water and used to calculate an effective diffusion coefficient of the bentonite in the buffer of 1.2×10^{-10} m^2/s, taking a porosity of 0.43. It is stated that future work needs to investigate the significance of using only a single diffusion coefficient. Is SKB addressing this issue?

On page 17. para 5 of TR-10-59 it is stated that the TOUGHREACT simulations used the thermodynamic database from the EQ3/6 software package, the most relevant minerals and species in which were checked for consistency with the data in SKB’s TRAC system (SKB-TDB). What is the meaning of “consistency” here? The implication is that the data for the relevant minerals and species in TOUGHREACT are similar to those in the EQ3/6 database. However, the EQ3/6 database is not actually internally consistent. Is the SKB-TDB also not internally consistent? Some comment about the potential significance of inconsistency in thermodynamic data for the modelling that has been undertaken would be helpful.

On page 19, Table 3-2 gives the composition of the bentonites that were used in the simulations of the buffer and backfill evolution. However, the compositions are slightly different to those given in the **buffer production report** (TR-10-15) and the **backfill production report** (TR-10-16). For example, TR-10-16 states that there is no pyrite in raw Milos bentonite. However, Table 3-2 of the report on **geochemical evolution of the near-field** (TR-10-59) states that this bentonite contains 1.5 wt% pyrite. Potentially, even small discrepancies like this one could make a significant difference to certain outcomes of the simulations.

Table 4-1 on page 24 of TR-10-59 gives hydraulic parameters that were used in modelling Case I and Case II. Several of these values are different to values given in other sources. The **data report** (TR-10-52) gives diffusion accessible porosity for neutral and cationic species in the buffer as 0.435 (best estimate), and for anions 0.174 (best estimate). For the backfill the figures are 0.46 and 0.184 respectively. These values compare with porosities in Table 4-1 of 0.43 and 0.44 for compacted buffer and backfill respectively. Similarly, according to the **data report** (TR-10-52) the dry density of the backfill in SR-Site should range between 1,458 and 1,535 kg/m^3, with a best estimate of 1,504 kg/m^3. The buffer for SR-Site should have a dry density within the range 1,484–1,640 kg/m^3, with the best estimate of 1,562 kg/m^3. These values are slightly different to the ones given in Table 4-1 of TR-10-59 of 1,570 kg/m^3 and 1,512 kg/m^3 for buffer and backfill respectively. While these small discrepancies will not be significant for the overall outcomes of the modelling, they do help to create doubt in the mind of the reader about communication of information between different parts of SKB's programme.

In TR-10-59, two model cases are evaluated:

1. Case I which simulated groundwater reaching the near-field through a pre-existing fracture that intersects a deposition hole and causes flowing groundwater to contact the bentonite buffer directly; and

2. Case II, which simulated a pre-existing fracture intersecting an access tunnel and movement of water though the fracture flows, the tunnel backfill and then the buffer in a deposition hole.

The simulations were undertaken for a period of 100,000 years. According to page 27, para 2 of the report on **geochemical evolution of the near-field** (TR-10-59) this interval was chosen because it is the minimum that performance assessments need to consider. However, there is no discussion of the implications of continuing the simulations for a period of 1 Ma, which is also considered by SR-Site.

In Case 1, as in most modelling of buffer evolution reported in the various SR-Site documents, the fracture is specified to intersect the deposition hole half way up.

The explanation of the 1-D modelling of buffer resaturation in Case I is difficult to follow. It is not clear exactly how the resaturation times were adjusted. On page 22, Table 3-5 states that water saturation in the bentonite buffer was achieved in different model runs after 10, 100, 1000, 2000 years for low advective flow in the fracture, and after 10 and 100 years for high advective flow in the fracture. What parameters were varied to achieve saturation after only 10 years (for example) when there was only low advective flow?

Page 25, para 8 of TR-10-59 states that "In the case that carbonate minerals are initially absent in the near-field (MX-80 bentonite), protonation of the montmorillonite surface is a well-known process that may have a relatively important role on the pH buffering". However, according to the **buffer production report** (TR-10-15) small quantities of carbonate minerals (calcite and siderite) could be present in MX-80. If so, then the pH buffering would be very different to that which would occur if surface protonation buffers pH. However, no comment is made about this possibility. In any case, it is stated in the same paragraph that "Protonation reactions have not been implemented in the numerical models developed for the thermal period due to limitations of the code TOUGHREACT used for these simulations. Therefore, protonation reactions are only taken into account in the numerical models of the water-saturated period performed with the code PHAST". No comment is made about the significance of this limitation of TOUGHREACT.

Page 25, para 10 of TR-10-59 states that "In order to develop a sensitivity analysis on the main parameters of the groundwater that enters the modelled domains through the hypothetical fracture of the granitic host rock…. the fracture-filling minerals have been neglected." The meaning of this statement is unclear. Does it mean that fracture-filling minerals were neglected in one specific alternative case, but included in other cases? How would the fracture filling minerals act to buffer the composition of inflowing (or out-diffusing) water? Some comment should be given.

On page 26, Table 4-3 states that Deponit CA-N bentonite contains 0.49 wt % pyrite. However, according to the **buffer production report** (TR-10-16) no pyrite occurs in this bentonite.

It is stated in page 27, para 5 that the groundwater at Forsmark is calculated to be oversaturated with respect to calcite and undersaturated with respect to pyrite, but the modelled Forsmark water is assumed to be at equilibrium with both minerals. This approach, without qualification, seems odd. Either the groundwater data used to calculate the mineral saturation states are incorrect, or the model is incorrect. Some comment should be given about the potential significance of the possible difference between the actual groundwater chemistry and the modelled groundwater chemistry. Additionally, the model outputs depend to a marked extent on the assumptions made concerning the saturation states of silica-bearing minerals. However, there is no discussion about these assumptions. On page 28, Table 4-7 states that .the groundwater contains1.85 x 10^{-4} mol/l Si, while MX-80, Deponit CA-N and Backfill contain 1.26 x 10^{-4} mol/l 1.27 x 10^{-4} mol/l and $1.26 \cdot 10^{-4}$ mol/l respectively. It is then stated in para 1 of page 29, that the bentonite porewater is equilibrated with respect to quartz. An implication is that the groundwater (which contains a higher concentration of Si) is oversaturated with respect to quartz. This situation is not unreasonable since low-temperature groundwaters typically have Si concentrations consistent with a control by amorphous, or poorly crystalline silica. However, it is not clear why the porewater in the bentonite could not similarly have Si concentrations buffered by amorphous or poorly crystalline silica.

Table 4-9 on page 31 gives alternative flowing groundwater compositions that were used in the sensitivity analyses for Case 1. To produce each alternative composition one parameter was varied (pH, C(IV) concentration, S(VI) concentration or Ca concentration) and some of the other parameters were allowed to vary depending on the alternative composition being specified: Cl varied according to charge balance; pH, HCO_3^-, SO_4^{2-} varied according to specified mineral equilibria,. If HCO_3^- was varied pH was constrained by calcite equilibrium in some compositions, but not all compositions. For other compositions, HCO_3^- was constrained by equilibrium with calcite, although not all compositions. If Cl^- and SO_4^{2-} were not varied independently, they were fixed by charge balance and equilibrium with gypsum respectively in some waters, and not in others. Apart from the small number of parameters that varied between alternative compositions, all other parameters were kept the same as the reference water composition in Table 4-7.

Unfortunately, TR-10-59 does not give the saturation states in the alternative water compositions of all the minerals that occur in the buffer, backfill and rock. There is an explicit mention only of those minerals that were used to constrain each water composition. Readers cannot easily interpret the calculated mineralogical changes presented later in the report, because the saturation states of the other minerals are unreported. For example, under higher-pH conditions, quartz (and other silica-phases) will become less supersaturated (or more undersaturated). Consequently, compared to the reference case, there will be variations in the calculated redistribution of quartz in the buffer during the thermal phase. It would have been helpful to present a table showing the mineral saturation states consistent with all the various initial water compositions. It would also have been helpful for Table 4-7 to present the Na/Ca ratios of the various water compositions.

Some of the outputs are actually artefacts of these alternative water compositions. Page 59, para 1 of TR-10-59 states that “The sensitivity analysis on the chemical composition of the inflowing water, performed for the flow rate of 10^{-3} m^3/yr, shows that when the concentration of aqueous carbonate of the inflowing groundwater is 10^{-2} mol/L (2.2×10^{-3} mol/L in the reference case), computed pH decreases from 7.19 to 6.63”. This change in the pH appears to be mainly a result of the fact that, in order to maintain equilibrium with respect to calcite, the alternative water composition with elevated HCO_3^- has a lower pH than the reference water.

On page 40, para 8 line 6 it is stated that “After 10 years the aqueous SiO_2 concentration decreases due to dilution provided by the inflow of the granitic groundwater which is depleted in SiO_2(aq) compared to the initial bentonite porewater.” This statement is inconsistent with the stated initial conditions and with Table 4-7 on page 28.

4.4.4. Cement-Bentonite Interactions

Models of cement degradation are provided in reports on **quantitative modelling of cement grout degradation** (TR-10-25) and **low-pH cement degradation in tunnel plugs and bottom plate systems** (TR-10-62). Report TR-10-25 concludes that alteration fronts in cement within grouted boreholes progress insignificantly under repository conditions for times up to 1,000 years (the time period considered). Report TR-10-62 concludes that low-pH concrete alteration would affect the stability of backfill materials to only a small extent.

The conclusions of both reports are reasonable and consistent with the findings of research carried out by other radioactive waste management programmes. However, the representations of chemical processes in the models described in TR-10-25 and TR-10-62 are inevitably very simplified compared to the processes that would actually occur. The reasons for the simplifications and their possible significance (or otherwise) would benefit from additional explanation. For example, the cement model in TR-10-25 appears to treat only CSH phases, silica, portlandite and calcite (which is not present initially, but which may form). The report recognizes that certain other minerals, such as ettringite, may form in the cement and reasonably points out that these omissions are a source of uncertainty. However, there is no comment about the potential significance of this uncertainty. Similarly, the models presented in TR-10-25 appear to include only a very simple representation of precipitation / dissolution kinetics for CSH and silica, although only rate constants and surface areas (for CSH only) are given. There are no details of the rate laws employed, or their implementation in the model. There is no discussion of the uncertainties associated with the representation of kinetics, although these uncertainties are acknowledged to exist. Is SKB undertaking a programme of work to assess the significance of these uncertainties?

Report TR-10-25 describes models of long-term grout evolution that represent solid solutions of CSH phases. Two solid solution models are evaluated, one by Carey and Lichtner (2007) and one by Sugiyama and Fujita (2006). While the reasons for evaluating the latter model are clear, since it is designed to represent CSH evolution over the full pH range of concern, it is unclear why the Carey and Lichtner model was chosen for evaluation, as opposed (say) to a modified Berner model.

The modelling reported in TR-10-25 found that the solid solution model of Carey and Lichtner (2007) can reproduce results of experimental cement degradation for Ca/Si ratios > 1, but cannot fit experimental data for so-called “low-pH cement”, with lower Ca/Si ratios. In contrast the model of Sugiyama and Fujita (2006) was found to reproduce experimental data for the full range of relevant CSH phase compositions. This solid solution model of Sugiyama and Fujita (2006) was then implemented in a reactive transport model of grout degradation. The model was used to simulate the interaction between groundwater in a fracture and grout in a borehole that is intersected by the fracture. A period of 1,000 years was simulated. Two 1D cases are described: (1) grout alteration due to diffusing groundwater; and (2) grout alteration due to advecting groundwater.

A key conclusion of TR-10-25 is that clogging of the porosity within the cement will quickly (within 100 years or so) cause any advective transport to cease. It is stated that consequently, all mass transport associated with long-term alteration of cement is expected to be dominated by diffusion. It would be helpful to note that the continuation of transport by diffusion implies that clogging is not complete in the sense that a small volume of connected porosity remains. This is a realistic assumption, but it would be helpful to state explicitly.

The conclusion that diffusive transport will quickly become dominant is reasonable, especially since the modelling did not represent certain secondary minerals, such as ettringite that could precipitate to occlude porosity. However, the predicted clogging will depend on the spatial discretization represented in the model. The finer the discretization, the quicker will be the clogging and the faster the system will cease to support advection. The discretization of the cement within the model is very fine (100 compartments over a distance of 10 mm for the 1D simulation. This fine discretisation will tend to enhance the predicted clogging, compared to a coarser discretization. There is also no discussion in the report of the possible significance of this relationship between discretization and pore space clogging.

The description of modelling in TR-10-25 would benefit from the inclusion of more details about the thermodynamic data that were employed. It appears that thermodynamic data for CSH were taken from the published descriptions in Carey and Lichtner (2007) and Sugiyama and Fujita (2006), as appropriate. The only mentions of any other thermodynamic data are in the caption of Figure 2-7 and a footnote to Table 3-3. The former states that the SKB-TDB was used to model aqueous speciation. The footnote to Table 3-3 states that some molar volumes were taken from Bourbon (2003). It would be helpful for further information to be provided about the suitability of the thermodynamic data for this modelling.

Report TR-10-25 is also unclear about the representation of silica in the cement. Presumably this was modelled as amorphous silica, but this topic appears not to be mentioned.

The models described in the report on **low-pH cement degradation in tunnel plugs and bottom plate systems** (TR-10-62) investigate interactions between groundwater, cement plugs / bottom plates and backfill. Although investigation of bottom plates implies that interactions between cement and buffer materials will be included in the modelling, in fact the models are stated to investigate explicitly only the contact between cement and backfill. Omitting consideration of buffer materials is not significant for the presented modelling in so far as the represented backfill is highly simplified. However, it does mean that the report does not explore possible differences in interactions between cement – backfill and cement – buffer, noting that backfills and buffers will have different compositions.

Section 4.2.2 of TR-10-62 states that “The backfill considered in this project is assumed to consist basically (69 wt%) of Milos-type bentonite. The mineralogical and physical properties are described in /Olsson and Karnland 2009/. Accessory mineral concentration is shown in Table 4‑3, and includes dolomite, quartz, calcite and gypsum”. The accessory minerals appear to account for about 11 wt% of the backfill, although Table 4-3 gives volume % mineral concentrations for the accessory minerals whereas the text gives wt% concentrations for the bentonite. It would be helpful to present a table of all the constituents of the backfill using consistent units. Presumably the remaining c.20 wt% of the backfill is silica (quartz?), although this is not mentioned. The only minerals that the model allows to precipitate in the backfill appear to be cement minerals, the primary mineral already present, ettringite and katoite. The representation of possible secondary minerals is therefore a very significant simplification compared to the mineral assemblages that could possibly form in reality. Zeolites, for example, are possible secondary phases within the backfill. However, there is no discussion of the possible significance of these other minerals, nor of the possible significance of excluding them.

The conclusion in TR-10-62 that alteration within the backfill will be very limited appears to rely on the modelled establishment of diffusion-dominated transport as a result of pore clogging. TR-10-62 used a coarser discretization than the 1-D models presented in TR-10-25. The regions within the cement within 2 cm of the cement’s boundaries were divided into cells representing widths of 1 mm. The central part of the cement was divided into cells representing widths of 10 mm. As noted above, the discretization will influence the calculated rate of clogging. However, there is no discussion of this relationship.

TR-10-62 represented reaction kinetics for all minerals. However, insufficient details are given about how this was done. Rate constants are specified without details of their sources and no details are provided about the rate laws that were implemented.

Like TR-10-25, TR-10-62 provides insufficient details about the thermodynamic data that were used. Appendix A.3.3 states that “We will use the thermodynamic database from SKB’s Trac system. Thermodynamic and kinetic data for cement minerals will be discussed and selected”. However, apart from CSH data taken from the solid solution model of Sugiyama and Fujita (2006), molar volumes (for CSH only) from Bourbon (2003) and molar volumes for calcite, dolomite, gypsum, silica and katoite in Table 4-2 (which are not attributed to a source), no data are given.

4.5. Computer Codes Used to Model EBS Evolution

4.5.1. General Comments on Computer Codes Used

The **model summary report** (TR-10-51) classifies the various computer codes used in SR-Site as follows:

> **Category 1** Commercial system software such as operating systems, compilers and data base software. It is noted in TR-10-51 that although necessary for the assessment, these codes are not regarded as assessment codes.
>
> **Category 2** Software used to solve problems that can be verified by simple hand calculations.
>
> **Category 3** Wide-spread commercial or open source codes.
>
> **Category 4a** Modified commercial codes.
>
> **Category 4b** Codes developed within the safety assessment, frequently written in languages like C++ and Fortran.

For commercial codes and widely-used open-source codes (category 3) and modified or bespoke codes (categories 4a,b) the most likely source of errors, if any, are in the use/application of the codes rather than the codes themselves or the models that they implement. For this reason it would seem important to include details in the **Model Summary Report** (TR-10-51) of the QA processes followed to ensure that input data files to models have been checked. For each individual modelling report in which a code (of any category) is used, relevant modelling verification examples should be presented where possible to demonstrate that the *calculation* (i.e. the application of the code) has been verified, rather than the code itself.

For commercial codes for which user-defined functionality/modules can be added to the code (category 4a) the additional likely source of errors, if any, is in these user-defined functions. Based on the review of TR-10-11, which uses Abaqus (a category 4a code), there does not appear to be a precise listing of the user-defined functions that have been added (they are only mentioned in passing), or any significant details of the QA checking for those routines. For example in TR-10-11, on page 214 it is simply stated that “The creep subroutines according to Equations (9-1) to (9-3) have been coded and verified.”, but no evidence supporting this verification is given.

It is suggested that a standard template could be included in modelling reports that make use of category 4a codes to allow user-defined functions to be precisely described and allow QA details to be recorded.

Category 2 codes are excluded from the QA considerations in the document (TR-10-51, page 14). For some of the types of software that is listed this is sensible, but for pre- and post-processing tools it is more crucial that some form of checking/QA has been performed. (It is possible that such checking is partly met by requirement 4 in Section 2.4 which refers to handling of input data that are transferred between codes, but it is not clear.)

In some cases it may be useful to obtain the input data/files that were used in the various modelling studies; e.g. to check that input data to models is consistent with data values in reports, or for model verification purposes. Are the input data files in the SKB archive freely available for this purpose?

4.5.2. Analytical Model

Section 3.3. of the **model summary report** (TR-10-51) describes analytical calculations to estimate the amount of buffer erosion and copper corrosion. These calculations are encoded in an Excel spreadsheet developed by SKB. The calculations to be performed are simple, being based on mass transport solutions using the Q_{eq} approach. Therefore a spreadsheet solution is appropriate.

The spreadsheet calculates an amount of corrosion for a single realisation of the DFN hydrogeological model. Statistical outputs based around multiple realisations of the DFN model are then performed using an additional script and the @Risk Excel add-in. Where results are to be used in radionuclide transport calculations, they are written to a dedicated sheet with a suitable format.

The @Risk add-in to Excel is widely used commercially available software and is appropriate for application to SKB's analytical model of corrosion. However, @Risk is not included in the list of software packages that are used in SR-Site. Since it is used to derive inputs for dose calculations, it is suggested that some justification for the use of @Risk (and its QA status) should be given in the **model summary report** (TR-10-51) in a dedicated subsection of Section 3.

The results of the model depend heavily on the input flow rates taken from the DFN calculations, which are a key factor in determining doses. It is assumed that the process by which DFN data has been processed for use in these calculations has been documented somewhere in the SKB bibliography. Is this assumption correct? If any significant processing of flow data is required then the technical specification of the calculations performed by the code should be reviewed.

The results of the model are also heavily dependent on any post-processing of the DFN output that has been performed to allow it to be used in the spreadsheet. Since the outputs on time for canister failure are direct inputs to the radionuclide calculations that underlie the dose calculations (**model summary report** (TR-10-51), Figure 2-1) it should be ensured that the flow rates from the DFN calculation are being used correctly and that any post-processing has been appropriately performed.

In the **corrosion calculations report** (TR-10-66), which describes the calculations performed in the spreadsheet, it is stated in particular that flow rates in spalling zones which are inputs to the model, are "calculated from the output of the hydrogeological DFN model" (TR-10-66, page 18). There are no details of how flows in the spalling zones are derived, which is a deficiency in the explanation. It is assumed that the spalling zones are not specifically represented in the DFN model and that some form of post-processing of the DFN outputs has been performed. Details of how these flow rates are calculated should be given and any pre/post-processing tools that have been developed for this purpose should be included in the Model Report. If they exist, any such tools would seem to be automatically excluded from QA consideration as they would belong to Category 2, but the reviewers suggest that they should not be excluded in this case.

Some investigation of the equations that are implemented in the spreadsheet have been performed (Section 5.1). This preliminary investigation would tend to suggest that the mathematical basis of some of the terms in the equations is possibly non-conservative. Additionally, the Q_{eq} terms that appear in the formulae are derived for idealised conditions (infinite plate solutions etc.) that are only an approximation to the relevant geometry in the buffer system. Although full derivations of these terms appear to be provided in the references quoted in TR-10-66 it is not clear that the accuracy of the approximation has been investigated, for example by comparisons with results obtained with other codes. Similarly, it is unclear whether their conservatism has been demonstrated. These topics should be reviewed as a separate task.

In summary, recommendations for improving the documentation of the analytical model are:

- The use of @Risk should by specifically documented by inclusion of a dedicated subsection of Section 3 giving justification for usage, version numbers that are used and information on the QA status of the code.
- It should be ensured that the flow rates from the DFN calculation are being used correctly and that any post-processing has been appropriately performed. This should be specifically reviewed as a separate task.
- In addition, details on how flow rates in spalling zones are calculated from the outputs of the DFN model should be provided. This should be specifically reviewed as a separate task. Any pre/post-processing tools that perform any significant calculations to derive these flow rates should be included in Section 3 of TR-10-51.
- The underlying formulae that are implemented in the spreadsheet calculation should be reviewed for their conservatism and accuracy of approximation to the variety of conditions that could arise in the backfill buffer system (e.g. with respect to variations in fracture intersect location, orientation and so on). See also the preliminary numerical investigation in Section 5.1.
- In general, pre/post-processing tools that perform any non-trivial calculations should be included in the list of codes in Section 3 of TR-10-51.

4.5.3. Code_Bright

Section 3.4 of **the model summary report** (TR-10-51) describes CODE_BRIGHT, which is used to simulate THM processes in the buffer, backfill and tunnel plug. The **model summary report** (TR-10-51) contains a good description of the areas in which CODE_BRIGHT has been applied in SR-Site. There are also references to the relevant modelling reports (**THM modelling report**, TR-10-11 and **cement grout degradation report**, TR-10-25), and thorough references to the suite of verification/validation documents for CODE_BRIGHT are provided. A useful high-level description of the system of equations that is implemented in the code is also given.

The code is by default of category 3, but some modifications to the code have been made that make it a category 4a code in instances where the additional functionality is used. Various versions of the code have been applied in SR-Site. One of the versions is “Version 3beta”. Since this would appear to be a beta release of the code the reader should be informed about the beta nature of the code. The **model summary report** (TR-10-51) should contain details of features of the code that are in “beta status” and a statement as to whether these have been fully tested and verified.

It is, however, clearly explained that the modifications to the software are not in the “foundation of the code” so that they should have no impact when the new constitutive laws are not used. Furthermore, the new features are described well in appendices C and D of the **THM modelling report** (TR-10-11), where details of testing of the new functionality are given.

In summary, the main recommendation concerning the CODE_BRIGHT model is that some additional clarification be provided on the beta nature of the

“Version 3beta” version of the code, within the **model summary report** (TR-10-51). It should be stated clearly whether or not any of the new ‘beta features’ used in the SR-Site modelling work have been fully tested and verified. If so, then details of the testing should be provided. Conversely, if not, then justifications should be given.

4.5.4. Abaqus

Section 3.2 of the the **model summary report** (TR-10-51) describes the Abaqus software. SKB sensibly justify their usage of Abaqus on the basis that it is an industry standard code that has been on the market for several decades.

Much of the material that is presented regarding capabilities of the code is directly taken from the Dassault Systemes website. It would have been helpful if more details on the applicability of the various capabilities of the code that are emphasised were given. For example, simulation of the interactions between ‘contacting bodies’ is described in traditional mechanical engineering terms, but the application to materials of interest in SKB’s EBS would have been useful.

Some apparently irrelevant information is given. For example, Abaqus/Aqua is described as being capable of simulating offshore structures such as oil platforms and the effect of wind loading. It would help the focus of the report if such irrelevant information was removed and more relevant examples should be given.

Abaqus is described as a Category 3 (widely-used commercial or open source code) and 4a (widely-used commercial or open source code with added modules / functionality) code. SKB sensibly point out that testing/verification of the core code is not deemed necessary. However it is important that any additional functionality that has been added to the core code to make it of category 4a is clearly identified and that quality assurance procedures are presented.

Other than to state that Abaqus is category 4a, no details of the functionality that is implemented by any extensions to the code are given. However, the **model summary report** (TR-10-51, Section 3.2.4) does state that:

“When user defined subroutines are used these have been verified by using simple test examples with known solutions (if possible) or by careful inspection of the obtained results.”

On inspection of **THM modelling report (**TR-10-11) the following statement is found:

“The finite element code Abaqus was used for the calculations. The creep subroutines according to Equations (9-1) to (9-3) have been coded and verified. For the swelling and consolidation processes Abaqus Standard has been used.”

Thus it would appear that the convention that is used is that details of the user-defined functionality are deferred to the detailed modelling report in which the functionality is used. This is sensible, but should be stated more clearly in **model summary report** (TR-10-51). Furthermore, in the excerpt from TR-10-11 above, no details/evidence of the verification of the subroutines is given.

In summary the following recommendations are made concerning the Abaqus code:

- No details on QA processes that have been undertaken to check the input data to the Abaqus models are given. It may be that this information is reported in the individual detailed modelling reports. However, it is recommended that this information should also be given in the **THM modelling report (**TR-10-11).

- The **THM modelling report (**TR-10-11) (and maybe others), which makes use of Abaqus, does not give a clear listing of all of the user-defined input subroutines that have been developed. It would be helpful to list these routines and reference accessible literature in which full details can be found.
- The **THM modelling report (**TR-10-11) (and maybe others), which makes use of Abaqus, does not have any information on checking/QA or an audit trail for the user-defined subroutines that are referred to in passing in the report. This audit trail should be provided in TR-10-11 and other reports that used Abaqus should then reference TR-10-11.
- The input data files used in the Abaqus calculations should be available for review if required in order to ensure a complete QA / audit trail.

4.5.5. TOUGHREACT

Section 3.21 of the **model summary report** (TR-10-51) describes TOUGHREACT. This software is a reactive transport and multi-phase flow simulator that was developed by adding chemical interaction capabilities to the TOUGH2 multiphase flow simulator. A good description of the areas in which TOUGHREACT has been applied in SR-Site together with references to the relevant modelling reports (**geochemical evolution of the near field** (TR-10-59), and **THC buffer modelling report** (TR-10-65)) are given. A high-level description of the system of equations that is implemented in the code is also provided that gives details of the couplings that are represented in the code between the flow and transport sub-problems. A list of the various equation-of-state modules that are available for use within TOUGH2 is given. Some of these are not especially relevant to the models constructed for SR-Site (e.g. those targeted at CO_2 storage), so it would be useful to clearly state the EOS modules that have been used.

The code is a category 3 code, being a widely used commercial code that is developed at LBNL. References to the TOUGHREACT User Guide are provided and the code’s wide use and publication history are suggested as evidence of checking/verification of the algorithms that it contains.

TOUGHREACT was used in the modelling of buffer evolution reported in the **geochemical evolution of the near field** report (TR-10-59). This report recognized that the inability of TOUGHREACT to model surface protonation reactions may be significant for the simulation of pH-dependent reactions. However, the wider implications of this limitation were not assessed.

In summary. it would be useful to state which of the EOS modules have been used in SR-Site.

4.5.6. PHAST

Section 3.18 of **the model summary report** (TR-10-51) describes PHAST, which is a reactive transport and single-phase flow simulator based on the PHREEQC and HST3D codes. A good description of the areas in which PHAST has been applied in SR-Site together with references to the relevant modelling reports, is given in the **geochemical evolution of the near field** report (TR-10-59). A high-level description of the system of equations that is implemented in the code is also provided. This description gives details of the couplings that are represented in the code between the flow and transport sub-problems. One coupling that is not specifically stated is that between the evolving porosity caused by mineral dissolution / precipitation and the flows that are calculated in the model (via changes in hydraulic conductivity); it would be useful to state whether this coupling is represented in the model.

The description of the code also usefully points out areas of application that the code is not suitable for (mainly unsaturated zone flows, and systems with concentrated solutions above 1 molal).

The code is a category 3 code, being a widely used open source code that is maintained by the USGS. Links to the PHAST website, which contains version control and verification details for the code, are provided.

It is recommended that it should be stated specifically whether the evolving porosity caused by mineral dissolution / precipitation is coupled to the hydraulic conductivity in the flow solve.

4.5.7. CRUNCHFLOW

CrunchFlow is used in a report on **modelling low-pH cement** (TR-10-62), which is cited in the **main report of the SR-Site project** (TR-11-01). The code was used to model low-pH bentonite cement interactions around the buffer bottom plate and tunnel plug. However, no details of CrunchFlow are given in the Model Report. Additionally, these interactions are not represented in the AMF (**model summary report**, TR-10-51, Figure 2-1). It appears that this is an omission.

4.6. Data for EBS Modelling

The **data report** (TR-10-52) does not contain all the data used, which is a significant deficiency in the documentation of the SR-Site assessment.

It would greatly help readers to understand other reports concerning the SR-Site assessment if all the data actually used were reported in a single document. Such a document should contain only the data, indications of associated uncertainties and references to data sources. In contrast the **data report** (TR-10-52) contains a lot of background information that is not needed for readers to understand other SR-Site reports. For example, there is much discussion of the SR-Can assessment. It would have been more appropriate simply to reference this information.

Some examples of where the data report has been found to be deficient are listed below:

Mineralogical composition of buffer / backfill

The mineralogical compositions of the buffer and backfill are not provided in the TR-10-52. Instead, references are made to the **buffer production report** (TR-10-15) and the **backfill production report** (TR-10-16).

Buffer / Package Dimensions

Buffer and package dimensions are shown in the illustrations on p16 of TR-10-52.

1. Total package height shown as 4.835 m in Figure 1-3
2. Total buffer height shown as 6.68 m in Figure 1-4.

3. Buffer above and below package shown as 1.5 m and 0.5 m respectively in in Figure 1-4.
4. So (2)-(3) implies a package height of 4.68 m, which is inconsistent with stated value in (1).

Backfill porosity variation with dry density

On page 142 of TR-10-52, the variation of porosity with dry density in the backfill is described as

”For the backfill, the porosities corresponding to the dry densities 1,458, 1,504, and 1,535 kg/m3 are estimated to 0.44, 0.46 and 0.48, respectively (Buffer production report, Table 6-2)”

The values of porosity listed in here would appear to be in reverse order.

Kd discussion

An important omission from Section 5.3.6 is a discussion of the nature and validity of the Kd concept and the limitations on its application.

Treatment of data uncertainty

Section 5.3.7 concerns the data uncertainties due to precision bias and representativity. However, again assumptions are often not clearly explained. Furthermore in some places data are recommended to precisions that are not really justified given the overall uncertainties. This is the case for diffusivities. In other places very broad statements are made about uncertainties without explaining their significance. For example, page 165 gives best estimate De values of 1.4 x 10^{-10} m^2/s for the buffer (ρ_d = 1,562 kg/m3) and 1.6 x 10^{-10} m^2/s for the backfill (ρ_d = 1,504 kg/m^3)”. Given that the difference between these values is small compared to the large scatter in the De data shown in Figure 5-6, it is unjustified to recommend different values for the backfill and the buffer. On the other hand on page 168 the first paragraph of the section entitled “Diffusion-available porosity” reports that published diffusion-available porosities for Cl are a factor of 1.8–3.5 smaller than for HTO. It is then proposed to use a reduction factor of 2.5 based on these data. However, the arithmetic mean of 1.8 and 3.5 is 2.65. Hence, why was a value of 2.5 recommended? While perhaps a minor issue, this case illustrates the inconsistent approaches adopted in this report when recommending parameter values for use in the assessment.

5. Scoping Calculations

In this section, some scoping calculations are presented that have been performed to check issues arising during the review. Details of more trivial calculations (mass balance calculations etc.) are given in the Section 0. More detailed independent modelling calculations of resaturation and homogenisation of the buffer are presented in Section 6.

5.1. Investigation of the Accuracy of the Buffer Concentration Factor (BCF) when Applied to Different Fracture Configurations

5.1.1. Description of Issues to be Checked

The Buffer Concentration Factor (BCF) term is used in TR-10-66 to represent the focussing of corrosion at locations on the canister surface closest to the fracture. This is described in the text accompanying TR 10 66 / Equation 4 19. The value of the BCF is taken to be 7, which is the maximum relative rate of corrosion that was derived from a sample calculation (SKI, 2006), in which it is assumed that the intersecting fracture with an aperture of 1 mm is located approximately mid-way along the canister height.

The accuracy/applicability of this estimate for other fracture configurations has not been demonstrated by SKB. Since it is used to compute the distribution of corrosion rates that is expected in the system, any under-estimation of this factor will lead to under-estimates in the probability distributions that are derived.

Results of calculations are presented that suggest the value of 7 for the BCF is not a sufficiently conservative value and would be likely to under-estimate the maximal corrosion rates when fractures are located away from the canister mid-height.

5.1.2. Description of Scoping Calculations

A model of mass transfer in a fracture-buffer system has been constructed using Quintessa's QPAC code (Quintessa, 2012), in which sulphide in the groundwater is transported to the canister surface from the groundwater in the fracture. The groundwater sulphide concentration has been set to SKB's maximal measured value of 1.2×10^{-4} mol/kg (TR-10-66, Section 4.3.5). A fracture with transmissivity of 10^{-7} m2/s and aperture of 1 mm has been assumed. This aperture corresponds to the extremal fracture aperture in the distribution of fractures in the Forsmark target area (TR-10-52 / Figure A-5) and is also the aperture that was considered in SKI (2006), in which the BCF value of 7 that is used by SKB was originally derived (as noted in the text near TR-10-66 / Equation 4-19). These parameter choices have been chosen to give rise to the maximum amounts of corrosion possible from the SKB dataset.

The geometry of the system that is modelled is shown in Figure 6. The location of the intersecting fracture can be varied in the model; the figure shows the intersection at the canister mid-height.

Due to the fast flowing nature of the fracture there is very little spatial variability in the corrosion profile on the canister surface, so in the results presented here the model is simplified to a constant sulphide boundary condition at the fracture intersection, allowing the solution to be calculated in (r,z) coordinates, which is the same assumption made in SKI (2006), where the BCF value of 7 was originally derived.

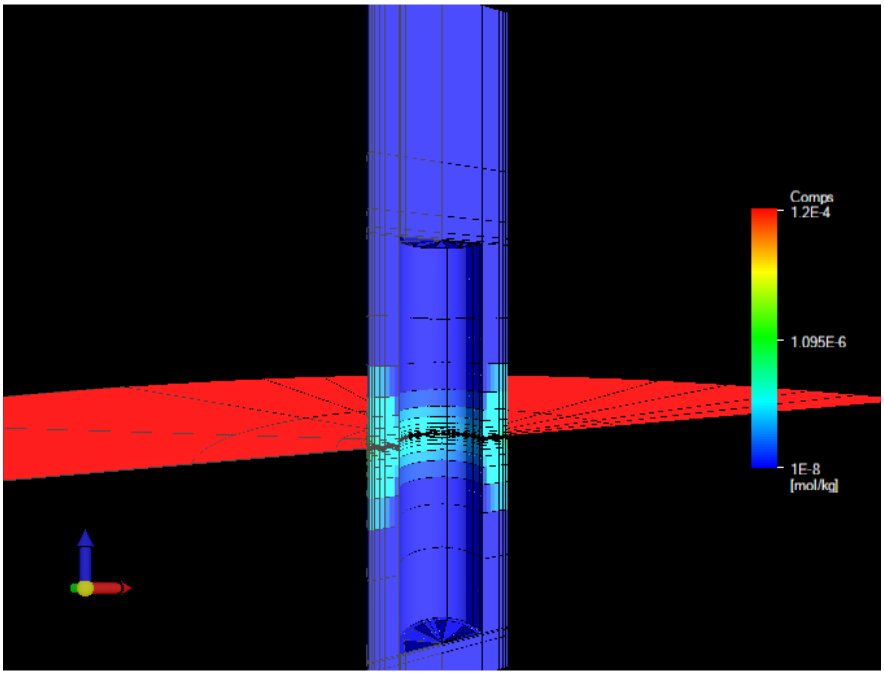

Figure 6 Geometry of the fracture/buffer system in which sulphide mass transport and corrosion was modelled. The location of the fracture can be varied in the model. Sulphide concentrations are shown by the colour scale.

5.1.3. Results from Scoping Calculations

Figure 7, Figure 8 and Figure 9 below show the corrosion depth profile and the derived BCF along the length of a canister from the example fracture intersect calculation. The position of the fracture intersection with the buffer is located at the canister mid-height in Figure 7 and at the canister top-height in Figure 8 and Figure 9.

For the case in which the fracture intersects at the canister mid-height (Figure 7), the computed BCF is around 7.05, which is consistent with the value of 7 calculated in SKI (2006).

The peak corrosion depth is clearly greater in the case where the fracture intersects near the top of the canister and the corresponding derived BCF is around 21 for the top of the side of the canister. In this latter case a similar depth of corrosion (2.5mm) is seen at the outer extremity of the canister lid, as shown in Figure 8, where the BCF is around 19.

It is noted that the average corrosion rate over the entire canister surface is similar in both cases, being controlled primarily by the transport of sulphide across the buffer-fracture interface.

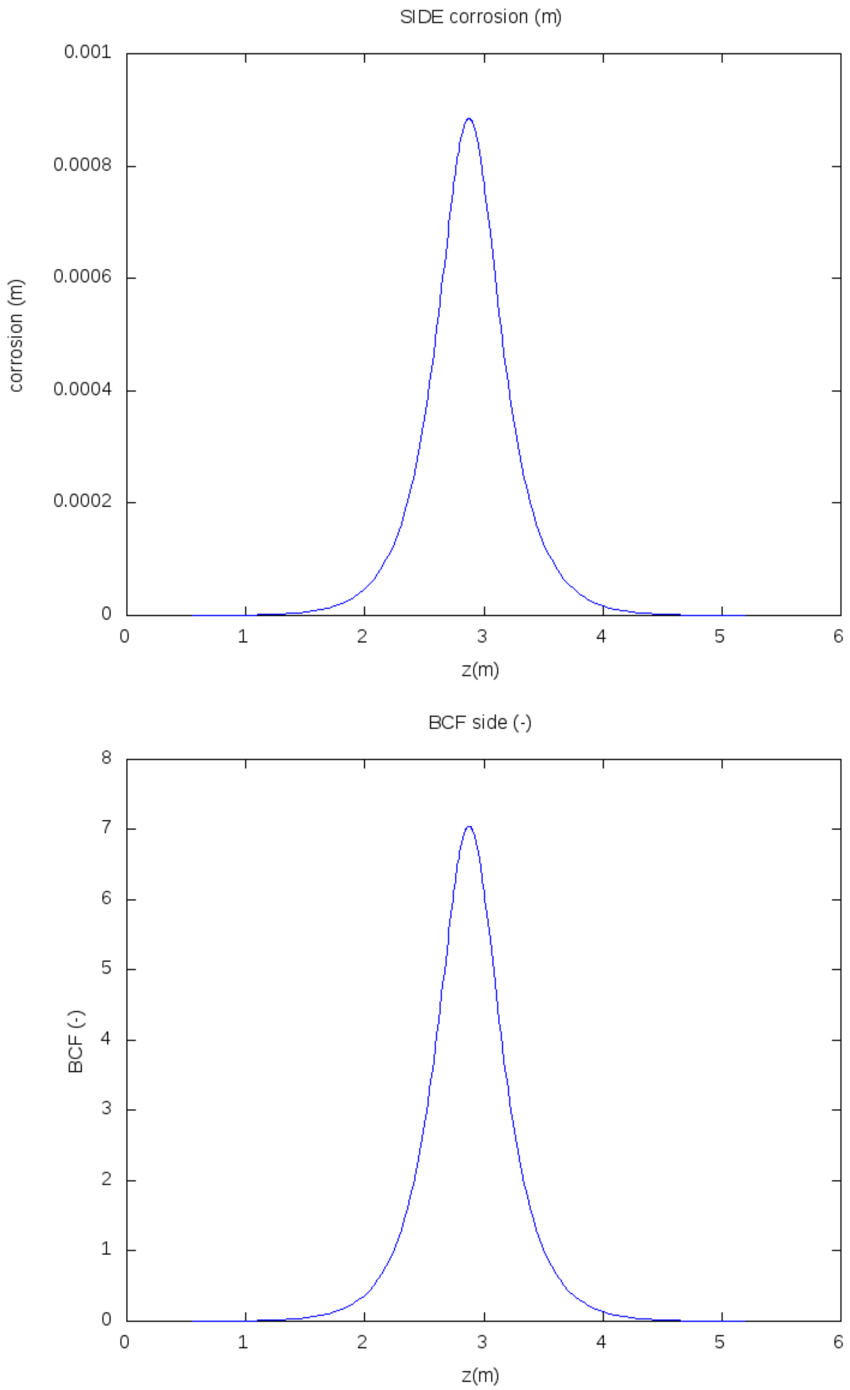

Figure 7 Corrosion depth calculation for fracture intersect at canister mid-height. Top – depth of corrosion along canister height (canister z range is 0.5-5.25); Bottom – derived buffer concentration factor

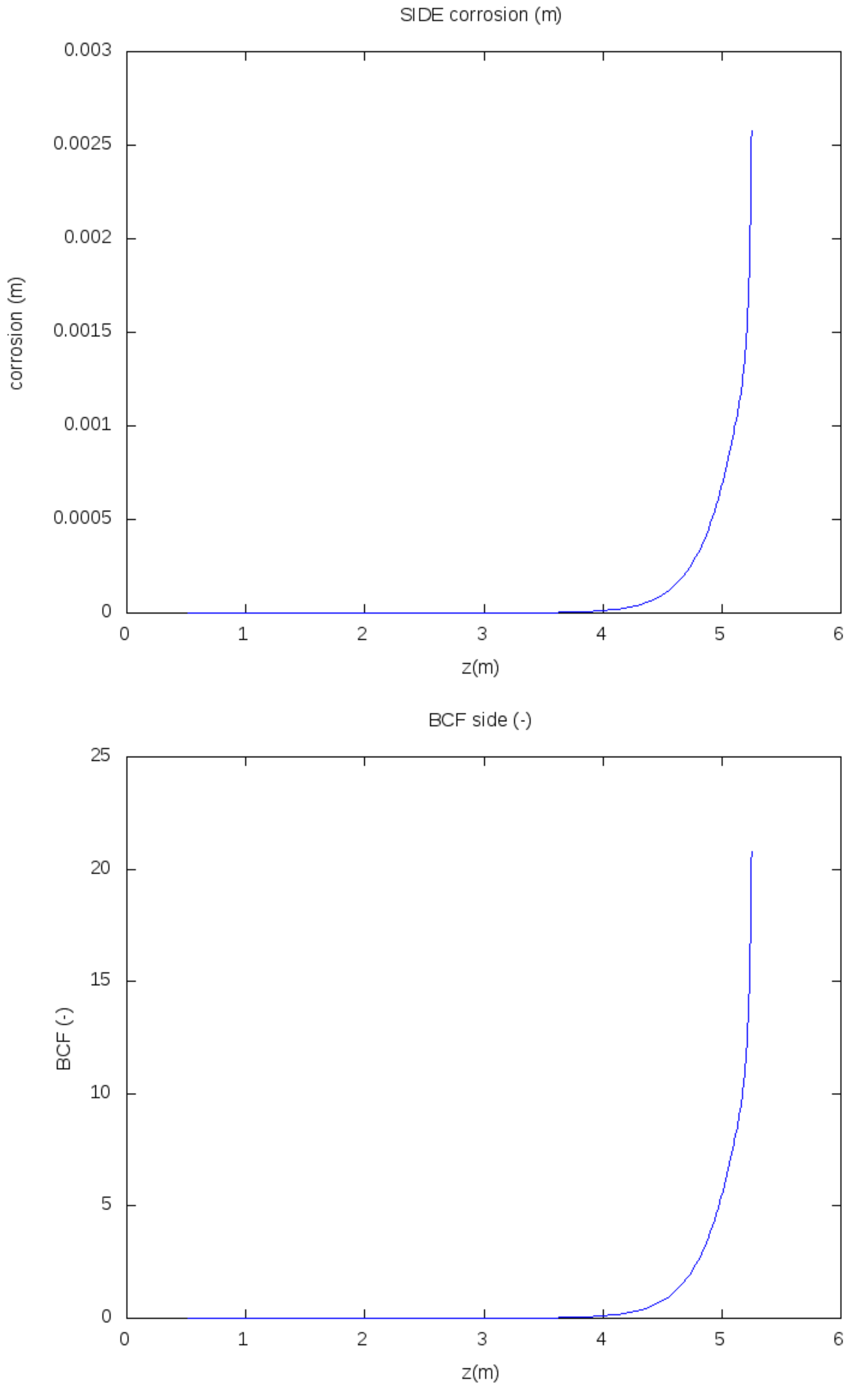

Figure 8 Corrosion depth calculation for fracture intersect at canister top. Top – depth of corrosion along canister height (canister z range is 0.5-5.25); Bottom – derived buffer concentration factor

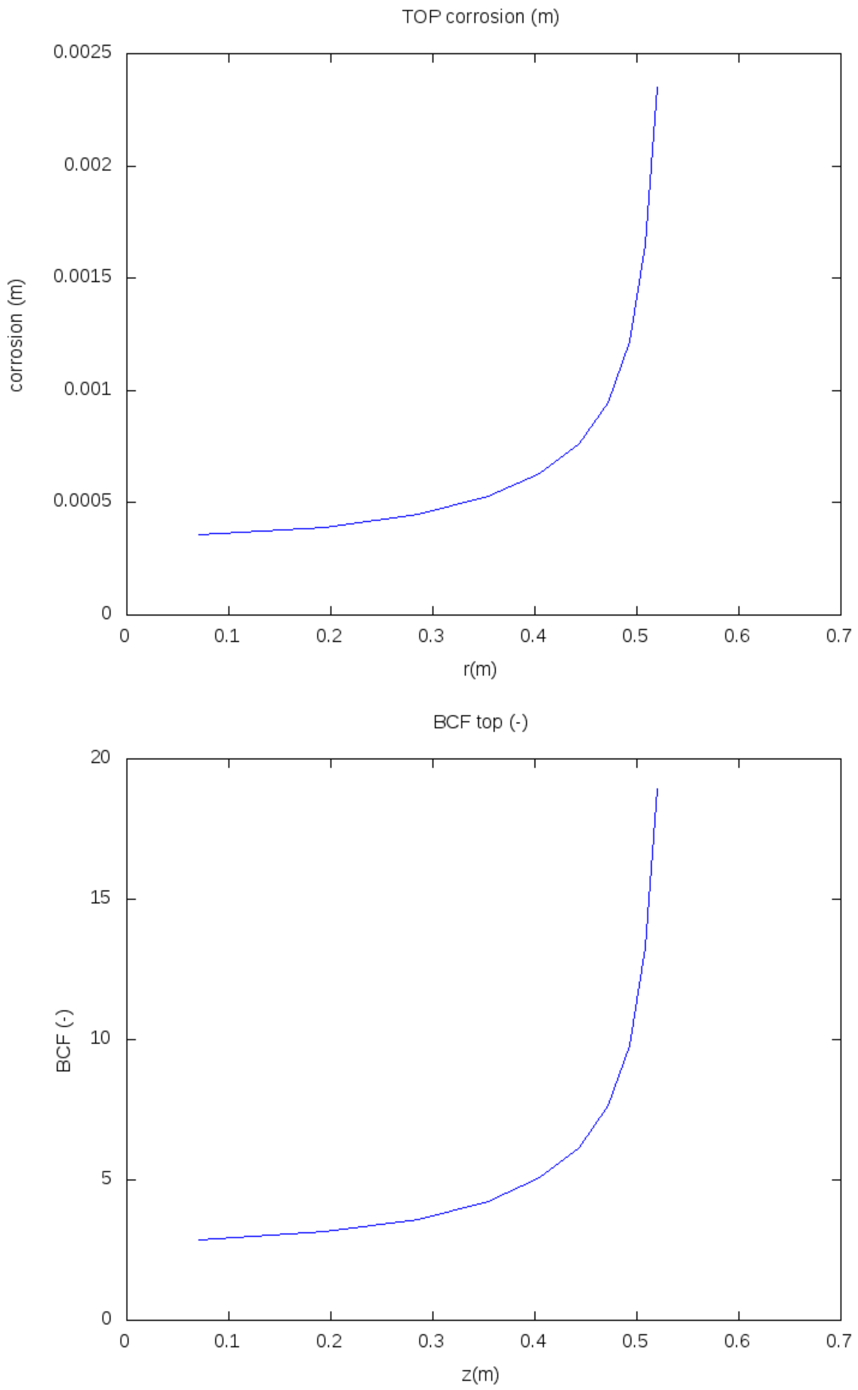

Figure 9 Corrosion depth calculation for fracture intersect at canister top. Top – depth of corrosion across canister lid; Bottom – derived buffer concentration factor

5.1.4. Conclusions of Scoping Calculations

The use of a fixed BCF of 7 would appear to under-estimate the maximum potential depths of corrosion due to ingress of corrodants in the Q_{eq} approach for configurations where the intersecting fracture is located away from the canister mid-height.

For example, Figure 10 shows the distribution of corrosion rates for the different geological DFN models calculated using the Q_{eq} approach (TR-10-66 / Fig 5-4). Superimposed on the plot are new datapoints corresponding to the results shown in Figure 8 and Figure 9. With the fracture assumed to be at the canister mid-height and with no spalling, the extremal value of the SKB distribution is attained for this choice of parameters (maximal sulphide concentration of 1.2×10^{-4} mol/kg and a fracture aperture of 1mm). For the same choice of parameters but with the fracture assumed to be at the canister top, the extremal value of the distribution is exceeded.

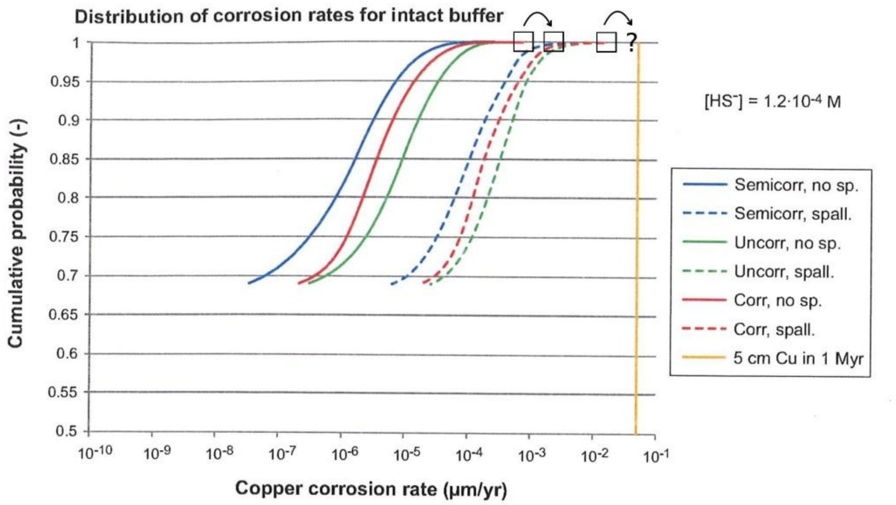

Figure 10 Reproduction of TR-10-66 / Fig 5-4 showing the distribution of corrosion rates for the different geological DFN models calculated using the Q_{eq} approach with new data points superimposed. From the left: the first square shows the corrosion rate corresponding to the fracture at canister mid-height calculation shown in Figure 7 (which coincides with the extremal point of the probability distribution calculated by SKB for holes without spalling); the second square indicates the corrosion rate from the calculation where the fracture is level with the top of the canister from the calculation shown in Figure 8 and Figure 9 (this is outside the bounds of the probability distribution calculated by SKB); the third square shows the extremal point of the probability distribution calculated by SKB for holes with spalling. Assuming that the spalling zone lies higher up the canister height may lead to increased corrosion rates than are predicted by the Q_{eq} model.

No modelling of the spalled zone has been included in this study. Without further modelling it is unclear whether SKB's use of the a BCF factor of 7 is appropriate in this setting, or how the BCF might scale if the spalled zone were to be located at different heights in the deposition hole. It is possible that for extreme choices of the parameter set it may be possible for the 5 cm of corrosion in 1 My target to be exceeded. This may not alter the overall risk estimates in SR-Site by a large amount, but nevertheless the analyses should acknowledge the possibility and properly capture the maximal potential rates of corrosion under the assumptions that have been made, which are currently being under-estimated due to the apparent inconsistency in the use of the BCF value.

It is noted that the BCF term is required in the SKB analysis due to the choice of using the Q_{eq} approach to calculate rates of corrosion of the package. Since this approach is generally only capable of calculating average corrosion rates across the canister surface, terms like the BCF (and other geometrical arguments) are used to derive scaled rates representing the corrosion rate at locations where the corrosion is more focussed.

Given the results of the calculations presented here, the following suggested future review and modelling tasks are suggested.

- A modelling study should be undertaken to properly assess suitable values of the BCF for different fracture configurations and that the estimates of corrosion.
- Due to the number of geometrical simplifications that need to be made in order to derive the analytical expressions for the various Q_{eq} terms at the key interfaces in the system, further work should be undertaken to verify the accuracy of the Q_{eq} terms for the range of geometrical configurations that might be present. This could be achieved by undertaking a thorough review of TR-10-42.

6. Detailed Review of a Selected Modelling Area

6.1. Introduction

Homogenisation of the buffer underpins a number of SKB’s safety functions for the buffer. According to the discussion in Section 8.3.2 of TR-11-01, the following safety functions of the buffer depend at least partly upon the premise that the buffer will be homogeneous:

- *Buff1:* Limit advective transport;
- *Buff2:* Reduce microbial activity;
- *Buff4:* Resist transformation; and
- *Buff6:* Limit pressure on canister and rock.

(See Section 4.1)

Homogenisation occurs by the redistribution of water within the buffer and by the redistribution of the bentonite mass itself. Water that is initially present in the emplaced bentonite blocks and pellets, and ingress water from the neighbouring rock and fractures, will be drawn through the buffer until a state of thermo-hydro-mechanical equilibrium is achieved. Longer-term geochemical interactions have the potential to alter the buffer and perturb its mechanical properties (for example as a consequence of porosity change and ion-exchange to less swelling forms), but the timescales associated with such changes are likely to be longer than the homogenisation period that is considered by SKB, where the overall duration is determined by the time taken for the buffer to resaturate.

SKB’s resaturation models of the buffer are TH models that are presented in TR-10-11 (Section 3). Differing assumptions of resaturation from: a sparsely fractured host rock; from a single discrete small fracture at the canister mid-height; and at the tunnel wall were considered. When resaturating from an individual fracture, cases with transmissivities that were set to provide 1% and 100% of the maximum allowed deposition hole inflow (0.1 l/min) were considered. (It is noted again that SKB do not appear to precisely define what is meant by this inflow rate and it is not apparent that the rate has been used consistently.)

In all cases, SKB’s models of buffer resaturation showed the buffer to resaturate fully (as characterised by all cells in the model having a water saturation greater than 0.99). In most cases, the timescale required for resaturation was less than 40 years, although for some low permeability sparsely fractured rock cases resaturation took up to 200 years (and 2000 years in a very low permeability case). See the discussion in Section 4.4.1 for more detail.

The TH models that SKB use in their resaturation study are calibrated against a THM model that was developed for investigating the Canister Retrieval Test (CRT) (Börgesson, 2007), in which the resaturation process was rapid. A collection of THM models are applied to the CRT dataset in TR-10-11 (Section 5), using both the Code_Bright (1-D) and Abaqus (1-D and 2-D) codes. It is assumed that one of the models presented there is the basis for the THM model used in the intercomparison with the TH resaturation models, although the precise THM model is not identified in the report. The THM models are shown to provide a good fit to many of the ‘homogenisation measurements’ from the CRT test, specifically a good fit was achieved to the evolved void ratio, suction and bentonite dry density, but not such a good fit to others such as the stress (which may be explained by the way in which the pressure sensors were installed).

It is clear that good models of the resaturation and homogenisation process are required in order to make reliable predictions of the rates of buffer resaturation that could be expected under in-situ repository conditions.

An independent model of the CRT experiment has been set up using Quintessa's QPAC code (Quintessa, 2012) in order to investigate the sensitivity of the predicted rates of resaturation and homogenisation to uncertainties associated with the (many) parameters in the model. Regarding these uncertainties, SKB note that

> *"The uncertainties are mainly the material models, which are very complicated, and the parameters values. Although they have been verified for the 1-D case of swelling and homogenisation of the bentonite rings and pellets between the canister and the rock, the 2-D case involves more degrees of freedom for the variables and more interactions like the friction between the bentonite and the rock or canister."*

Only a 1-D model has been considered in this short modelling study, the construction of which is similar to that of the 1-D Code_Bright model used by SKB. The outputs of the model have been directly compared to SKB's model outputs and to a number of measured quantities in the CRT dataset, including some not directly used by SKB.

The objective of the modelling is to both:

- Identify behaviour in the model that is sensitive to the choice of parameterisation and the underlying uncertainties; and
- Identify behaviour in the model that is known (from the CRT data) to be sensitive to parameterisation, but which is not necessarily reflected in the modelling outputs.

The former of these objectives will help to identify the effect that uncertainties in bentonite properties are likely to have on the predicted bentonite behaviour (if the model is to be believed) and help to illustrate the degree of confidence that is needed in the data values in order to be confident that the results are robust to uncertainties, whilst the later objective will help to illustrate areas in which the model cannot necessarily be relied upon to make firm predictions. These observations will only directly apply to the QPAC model from which they are derived, however for instances where there is seemingly good agreement between the QPAC and Code_Bright models the conclusions may also be relevant to SKB's models.

The structure of this Section is as follows: in Section 6.2 the QPAC CRT model is introduced; in Section 6.3 the QPAC model outputs are compared to the measured CRT data and the outputs of SKB's CRT models; in Section 6.4 the sensitivity of the model outputs to the chosen bentonite properties is investigated; and in Section 6.5 the sensitivity to the rock (hydraulic) boundary condition is assessed. Conclusions and questions that arise from the modelling are presented in Section 6.6, together with suggestions for issues that could be investigated in future.

6.2. QPAC CRT Model

6.2.1. Background

The calculations in this section are based around a fully-coupled 1-D model of the Canister Retrieval Test (CRT) developed for the THERESA project, implemented in Quintessa's QPAC code (Quintessa, 2012). The model has been updated from the original version reported by Bond et al. (2009) to be compatible with the latest versions of the QPAC thermal, mechanical and multiphase flow modules. A prototype 3-D model is also available but these preliminary calculations are based on the 1-D model.

A brief summary of the model is given below; full details can be found in Bond et al. (2009).

6.2.2. Processes

The process modules used in the QPAC THERESA model are as follows:

- Thermal. Includes processes of conduction, convection and radiation of heat. Details are given in Bond (2010).
- Multiphase Flow. Represents flows in porous media of water and other fluids. Various standard models are available for representing characteristic hydraulic functions, but algorithms specific to bentonite have been employed here. Full details of the module are given in Bond and Benbow (2009).
- Mechanical. Represents visco-elastic deformation of fluid-filled porous media, including swelling, thermal expansion and grain deformation effects. Details can be found in Bond et al. (2009).
- Porosity. A general-purpose porosity model for solid material mass conservation, including thermal expansion and stress effects. Details can be found in Bond et al. (2009).

6.2.3. Geometry

The geometry used by SKB for the 1-D Code_Bright simulations (TR-10-11, Section 3) is shown below in Figure 11. The location of the block/pellet interface (and thus the width of the pellet slot) does not quite agree with the specification of the CRT given in Thorsager et al. (2002); there the interface is reported as being at a radial distance of 820 mm, rather than 825 mm. However this discrepancy is unlikely to affect the results greatly. The QPAC THERESA model has been updated to use the same geometry.

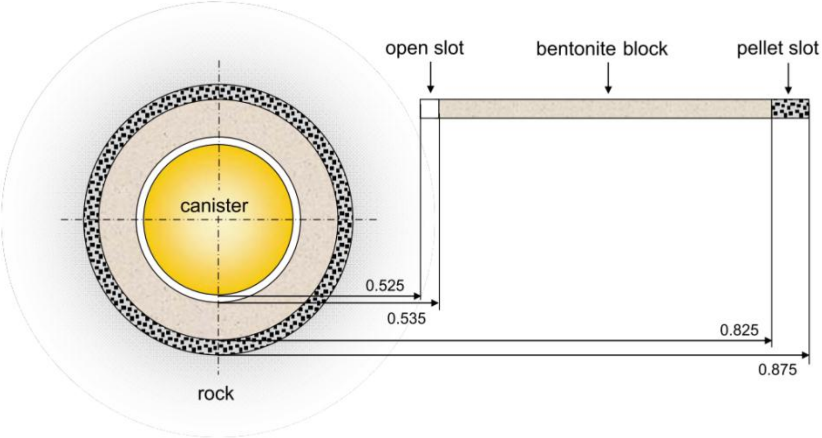

Figure 11: The geometry of the 1-D model (reproduced from Figure 5-16 of TR-10-11). Lengths are given in metres.

Unlike the Code_Bright model, the QPAC model does not explicitly include the open slot within the model domain. Instead it is treated as a boundary condition along with the rock.

6.2.4. Initial Conditions

The initial conditions for the model are based on the specification for the CRT given to the THERESA participants (THERESA, 2008) and are given in terms of the temperature, T, the water saturation, S, the total stress, σ, and the porosity, θ. The values used are given in Table 3.

Table 3: The initial conditions used in the base case model.

Medium	Thermal	Hydraulic	Mechanical
Bentonite ring	T = 20°C	S = 0.859	$\sigma = 0$, $\theta = 0.36$
Bentonite pellets	T = 20°C	S = 0.895	$\sigma = 0$, $\theta = 0.64$

6.2.5. Boundary Conditions

The boundary conditions applied to the model are described in Table 4. The non-calculated values are based on the CRT specification in THERESA (2008). Although the model is nominally 1-D, top and bottom boundary conditions are included to allow vertical upward displacement of the swelling bentonite. No flow is permitted through these boundaries.

Table 4: The boundary conditions used in the modelling.

Boundary	Boundary Condition		
	Thermal	**Hydraulic**	**Mechanical**
Air gap adjacent to canister	Time-varying temperature from experimental data	Specified pressure and saturation calculated from bentonite swelling	Specified normal stress, calculated from bentonite swelling; roller shear conditions
Rock wall	Time-varying temperature from experimental data	Time-varying pressure from experimental data; full saturation	Zero normal displacement; roller shear conditions
Top horizontal	No flux	No flux	Specified normal stress, calculated from bentonite swelling; roller shear conditions
Bottom horizontal	No flux	No flux	Zero normal displacement; roller shear conditions

The treatment of the inner boundary between the bentonite and the air gap adjacent to the canister is one of the key features of the calculations. It is assumed to be initially full of water, though there is some uncertainty over the degree of saturation of this gap in the experiment. As the bentonite swells and presses into the air gap the saturation is reduced, until it reaches zero when the bentonite touches the canister. At this point the boundary becomes no-flow.

The stress on this boundary is assumed to be equal to atmospheric pressure until the bentonite comes into contact with the canister, at which point it becomes a resistance boundary with a stress proportional to the excess displacement.

6.2.6. Parameterisation

A list of the parameters used in the model is given in Table 5, along with the source of information. In some cases values have been assumed; in others values are used as calibration parameters.

Table 5: List of input parameters used in the base case.

Parameter	Units	Value	Source
Acceleration due to gravity *g*	m s^{-2}	9.80665	Gettys et al. (1989)
Young's Modulus (Bentonite) *E*	MPa	150 (Rings) 1.5 (Pellets)	TR-00-14 with calibration

Parameter	Units	Value	Source
Poissons Ratio (Bentonite) v	-	0.3	Gens (2007)
Viscosity (Bentonite) μ	Pa s	0 (Creep disabled)	Assumption
Reference Porosity (Bentonite) θ_0	-	0.36 (Rings) 0.64 (Pellets)	THERESA (2008)
Initial Stress (Radial)	atmosphere (bar)	0	THERESA (2008)
Initial Stress (Vertical)	atmosphere (bar)	0	THERESA (2008)
Initial Water Pressure	atmosphere (bar)	1	THERESA (2008)
Elastic Response Time	years	1.0e-5	Assumption
Saturated Swell Pressure σ_{sat}	MPa	exp(6.77*ρ_d /1000 [kg/m^3]-9.07)*1[MPa]	THERESA (2008) (ρ_d = bentonite dry density)
Porosity Reduction Factor	-	0 (Ring) 0.75 (Pellets)	Assumed that in compacted bentonite all swelling goes into net volume expansion, while in the pellets the swelling dominantly acts to reduce the secondary porosity.
Stefan's Constant	W m^{-2} K^{-4}	5.6704e-8	Gettys et al. (1989)
Initial Temperature	degrees C	20.0	THERESA (2008)
Specific Heat Capacity c	J kg^{-1} K^{-1}	$(c_l*w*(1-r)+c_v*w*r+c_b)/(1+w)$ c_l = SHC of liquid water (4181.3 J kg^{-1} K^{-1}) c_v = SHC of water vapour (1850 J kg^{-1} K^{-1}) c_b = SHC of bentonite (800 J kg^{-1} K^{-1})	Linear scaling from value for dry bentonite to that of liquid H_2O w = water content (ratio of liquid to solid by weight) r = fraction of water as vapour
Thermal Conductivity Γ	W m^{-1} K^{-1}	$1.28-0.68/(1+\exp((S_w-0.65)/0.1))$	(S_w = water saturation)
Reference Water Density	kg m^{-3}	1000	Assumption

Parameter	Units	Value	Source
Reference Water Pressure	atm	1	Assumption
Relative Permeability $k_{r,i}$	-	(Water Saturation)$^{7/2}$	Calibrated from Claesson & Sällfors (2005) value
Intrinsic Permeability k	m^2	2.5x10^(-22+10(θ-0.2))	Derived from data in THERESA (2008) and calibrated (θ = porosity)
Reference Vapour Diffusivity D_v	$m^2\ s^{-1}$	2.5e-6	Claesson & Sällfors (2005)
Suction Pressure	MPa	10^6 exp(a-bw) [Pa] a= 7.25 (Ring), 6.3 (Pellets) b =21.1 (Ring), 14 (Pellets)	THERESA (2008); value of b calibrated. Expression for pellets moves towards that for bentonite ring as pellets swell. (w = water ratio)
Initial Water Saturation	-	0.859 (Ring) 0.895 (Pellets)	THERESA (2008)
Dry grain density ρ_m	kg m^{-3}	2780	THERESA (2008)
Fraction Bound (function of Water Saturation)	-	Linear interpolation using the following values: 0.999 at 0.0; 0.995 at 0.5; 0.992 at 0.7; 0.99 at 0.9; 0.95 at 1.0.	Calibration Parameter
Thermal Stability (function of Temperature)	-	Linear interpolation using the following values: 1.0 at 270 K; 0.95 at 280 K; 0.85 at 290 K; 0.85 at 300 K; 0.55 at 310 K.	Calibration Parameter

Note that in the mechanical module the angular convergence component of the strain was turned off. If the bentonite behaved as a hard material it would gain some circumferential strain as it was pushed radially inwards, resulting in it pushing back.

However bentonite can behave more like a fluid in which case this effect is reduced, justifying turning this component off.

6.3. Comparison with CRT and SKB Model Data

The base case results fit the experimental data reasonably well and provide a good match to the SKB results, even though a less sophisticated mechanical model is used in the QPAC model (the SKB model implements the Barcelona Basic Model (BBM) for the mechanical response of the bentonite). The axial stresses in the bentonite at radial distances of 585 mm, 685 mm and 785 mm are shown in Figure 12; the results of the independent calculation, like the SKB results, are higher than the experimental results, but the two models predict stresses of similar magnitude. As discussed in Section 5.5.2 of the THM modelling report (TR-10-11), the space around the sensors was packed with bentonite powder which may have affected the measurements; however the 1-D nature of the model also means that stresses are not properly represented. Both the models predict lower stresses in the bentonite pellet region (blue curve, also seen in the experimental data) but the SKB model suggests a larger disparity between the pellets and the bentonite ring.

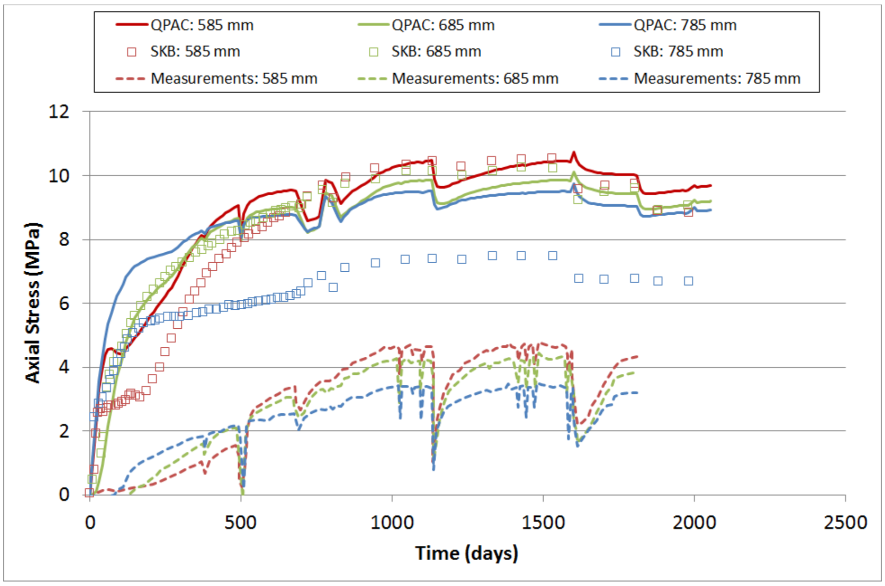

Figure 12: The axial stress at 3 points in the bentonite. CRT data (dashed lines) and SKB results (symbols) reproduced from Figure 5-22 of TR-10-11.

The void ratio profile at the end of the simulation is shown in Figure 13 along with the SKB results and the experimental data (both actual measured data and the SKB adjusted data). The independent calculations agree well with the data. There is a step increase in void ratio between the bentonite ring and the pellets in the independent calculations which is an artefact of the simple elastic model employed.

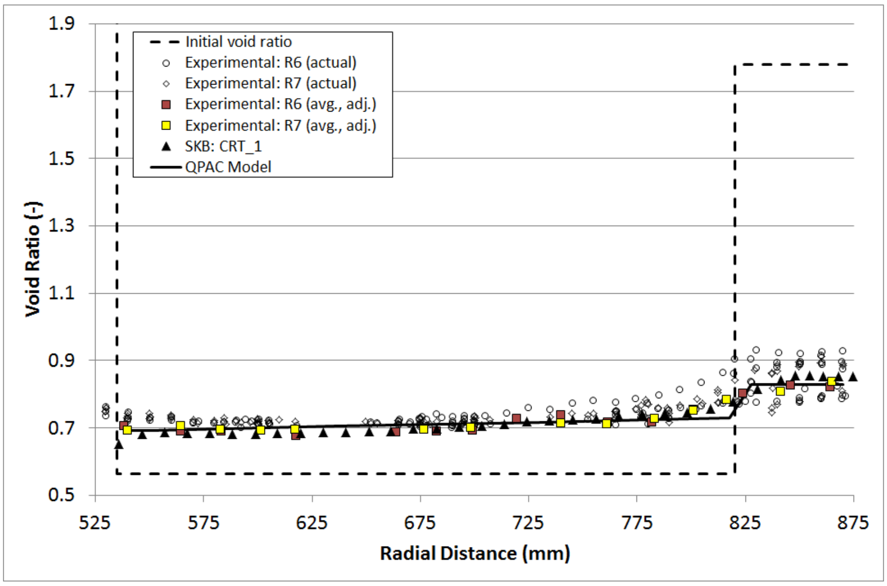

Figure 13: The void ratio profile through the bentonite at the end of the simulation. SKB results (filled triangles) and adjusted data (coloured squares) reproduced from Figure 5-21 of TR-10-11. Actual data (hollow symbols) reproduced from Figures 5-12 and 5-13.

The suction pressure at 3 different points in the bentonite is shown in Figure 14. There is good agreement between the independent calculation, the best-fit SKB model and the measurements.

The magnitude of the long-term residual suction that is reached is controlled by the parameter b in the expression used for the retention curve in the bentonite:

$$S_{free}(w) = 10^6 \exp\left(a - bw\right)$$

where w is the water ratio and a is another parameter. Both parameters a and b depend on the initial water ratio; values of 7.25 and 20 respectively are suggested by Dueck (2007) for an initial water ratio of 0.175 (close to the initial water ratio of 0.171 in the bentonite rings). A better fit to the data was found if b was taken to be equal to 21.1 in the model.

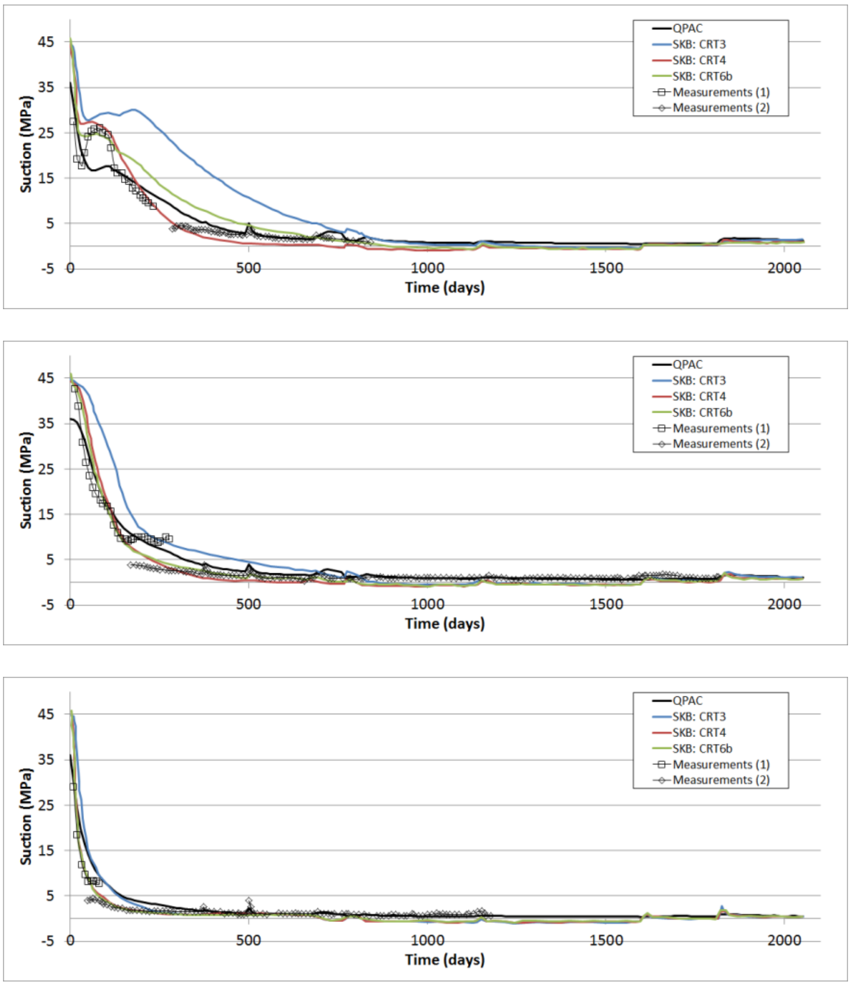

Figure 14: The suction pressure evolution at 3 points in the bentonite; 585 mm (top), 685 mm (middle) and 785 (bottom). SKB results and measurements reproduced from TR-10-11 (Figure 5-26).

Traces of the void ratio plotted against the net mean stress are shown in Figure 15 (original SKB results for 2 variant cases) and Figure 16 (independent calculations) for five different points in the bentonite. In both models, the trace in the pellet section follows a different path than that in the ring section due to the higher starting void ratio. In the SKB model all traces end up in the same region, but there is a larger difference between the finishing points of the pellet and ring points in the independent results, but the net mean stresses attained in the block regions are similar in magnitude to SKB’s.

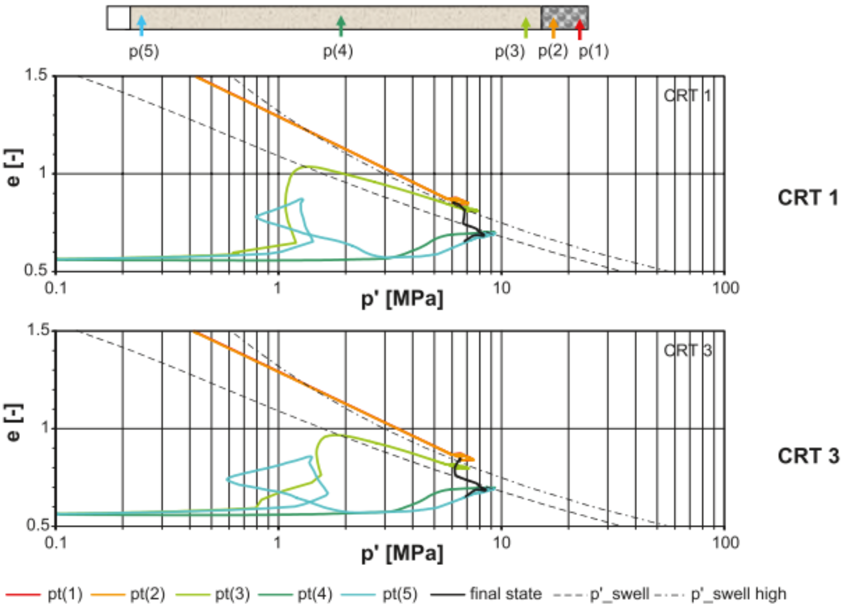

Figure 15: The void ratio plotted against the net mean stress for 5 points in the bentonite (locations shown in diagram above plot) – SKB results. Reproduced from TR-10-11 (Figure 5-23).

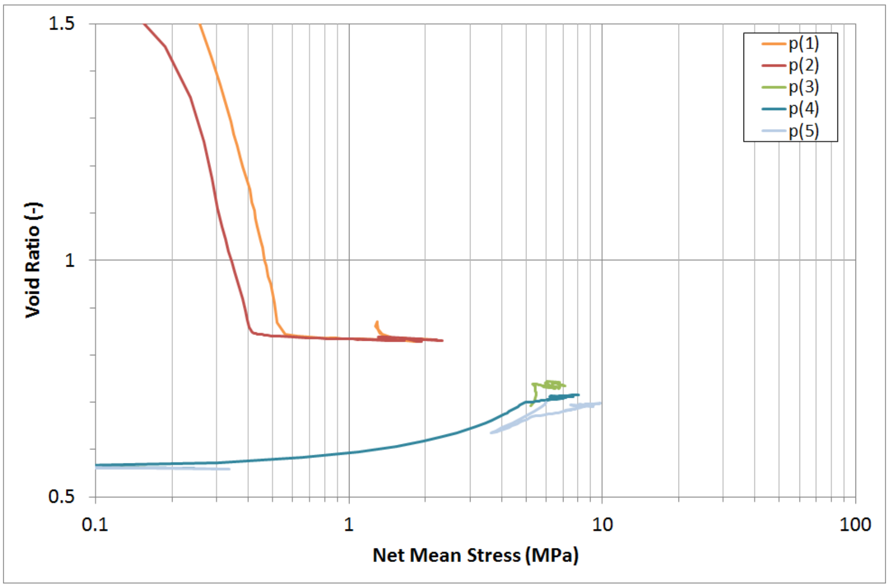

Figure 16: The void ratio plotted against the net mean stress for 5 points in the bentonite (see Figure 15 for locations).

Water saturation evolution plots for 3 different points in the bentonite are shown in Figure 17. The SKB model data is from TR-10-11 Section 3 where the 'THM CRT' model is compared against two TH models, as part of the calibration / justification for the use of the TH models in computing the resaturation timescales for the buffer. The independent QPAC calculation results are similar to the SKB

THM CRT model results. In each case full saturation is achieved within a few years.

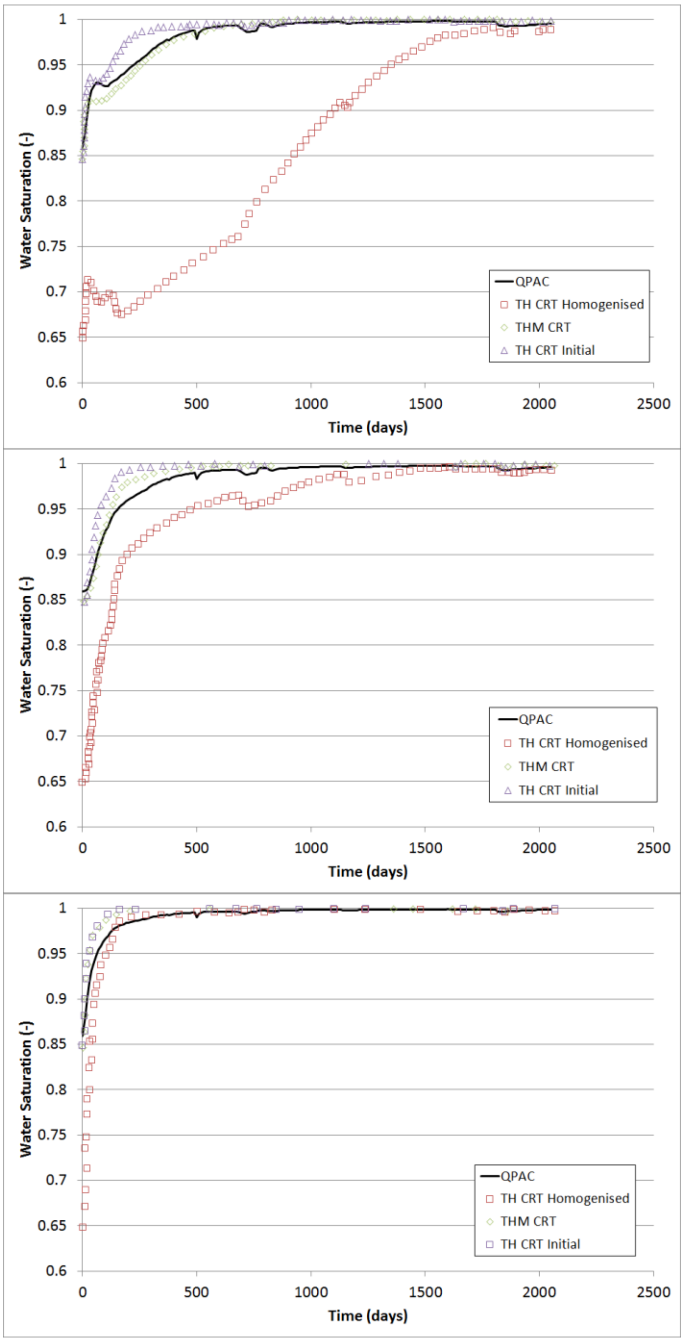

Figure 17: Resaturation evolution at 585 mm (top), 685 mm (middle) and 785 mm (bottom). SKB results (symbols) reproduced from TR-10-11 (Figure 3-9).

The water saturation profile across the bentonite at the end of the experiment is shown in Figure 18. Experimental data is included on this plot together with the corresponding QPAC output but no SKB model data is included since a corresponding saturation profile for the SKB models is not presented in TR-10-11. The resaturation data from the SKB model for the three points in the buffer in Figure 17 suggest however that a similar profile to the QPAC result would be obtained, since each of the three locations are close to, or at full saturation by the end of the experiment. The experimental data indicates that the bentonite nearest the canister did not achieve full saturation, with measured saturations are low as 0.92 in some locations (from an initial emplaced saturation of 0.85). None of the models exhibited this behaviour.

It is noted by Bond et al. (2009) that measurements of water saturation are considered to be less reliable than those of water content since they require information on the sample volume, which changes as the sample is unloaded. However the trend in the measured data as the canister surface is approached is clear, even if the precise saturation values cannot be relied upon. It is noted that if the bentonite rings adjacent to the canister surface did not achieve full saturation over the timescale of the experiment, then it would seem unlikely that the 'deeper' points towards the centre of the bentonite cylinders above and below the canister would have achieved full saturation over the experimental timescale.

The water ratio profile measured at the end of the experiment is shown in Figure 19 along with the independent calculation results, and does not show a decrease near the canister. The model results agree well with the experimental data in this case. The water ratio (ratio of water to solid by mass) is higher in the pellets than the bentonite ring whilst the water saturation is lower; as can be seen in Figure 20, the dry density is also lower indicating there is less solid mass and more porosity.

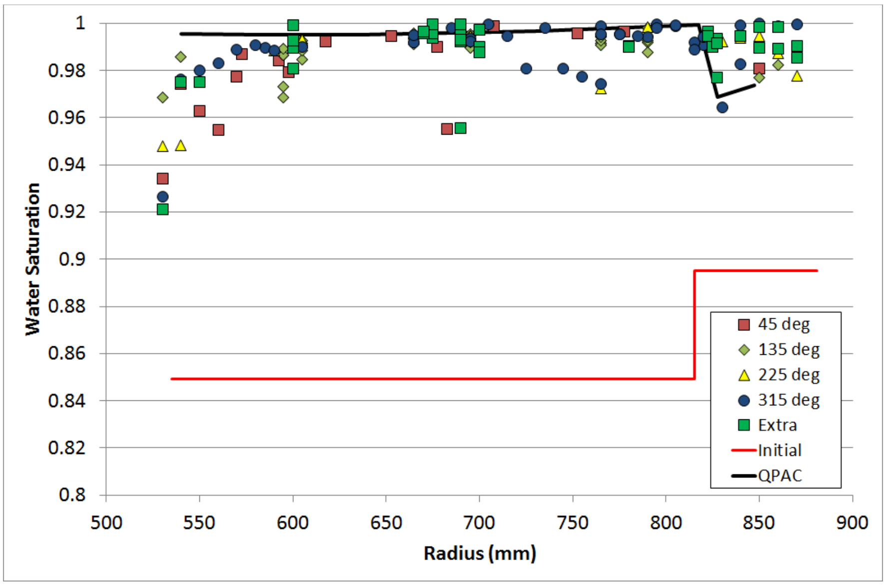

Figure 18: Profile of the water saturation through the bentonite at the end of the simulation. Experimental data (symbols) provided through the THERESA project.

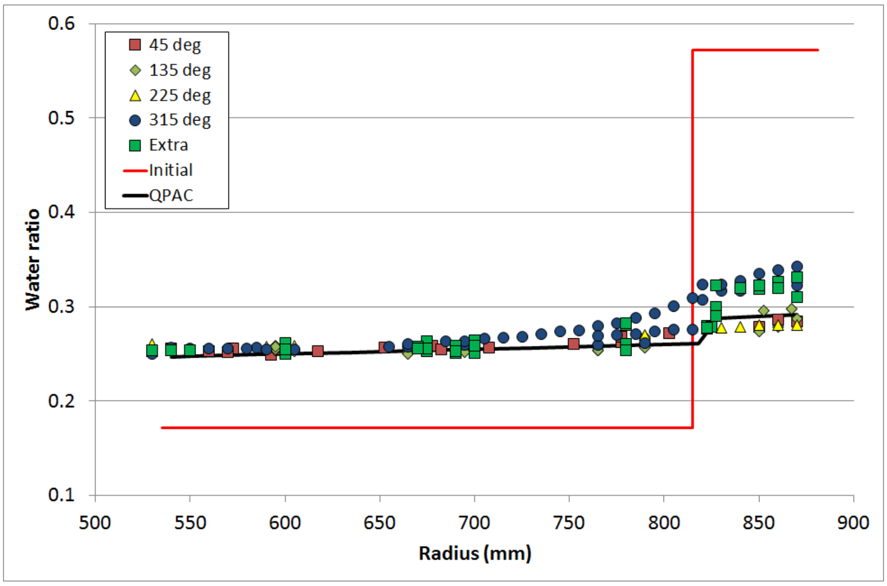

Figure 19: Profile of the water ratio through the bentonite at the end of the simulation. Experimental data (symbols) provided via the THERESA project.

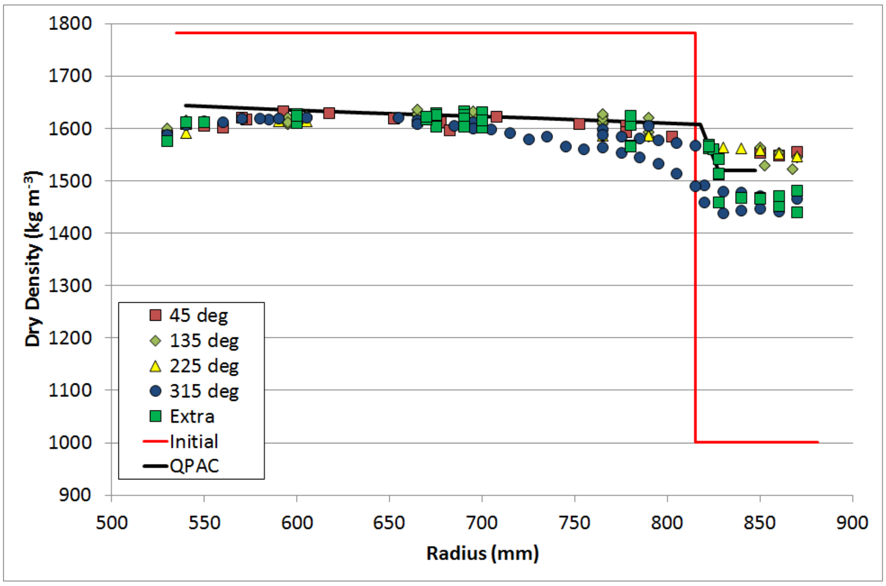

Figure 20: Profile of the dry density through the bentonite at the end of the simulation. Experimental data (symbols) provided through the THERESA project.

Two other measurements not presented by SKB are the temperature and relative humidity evolution, here shown in Figure 21 and Figure 22. In both cases the model results can be compared to the experimental data at various points through the bentonite. The temperature data does not extend through the whole period of the test, but an excellent match is obtained in the first 2 years with agreement to within 5 degrees in the latter stages.

The relative humidity is more difficult to match, as shown in Figure 22. However, the general trend is reflected by the model even though the detailed fluctuations, which correlate with the time-dependent heat source, are not captured so well.

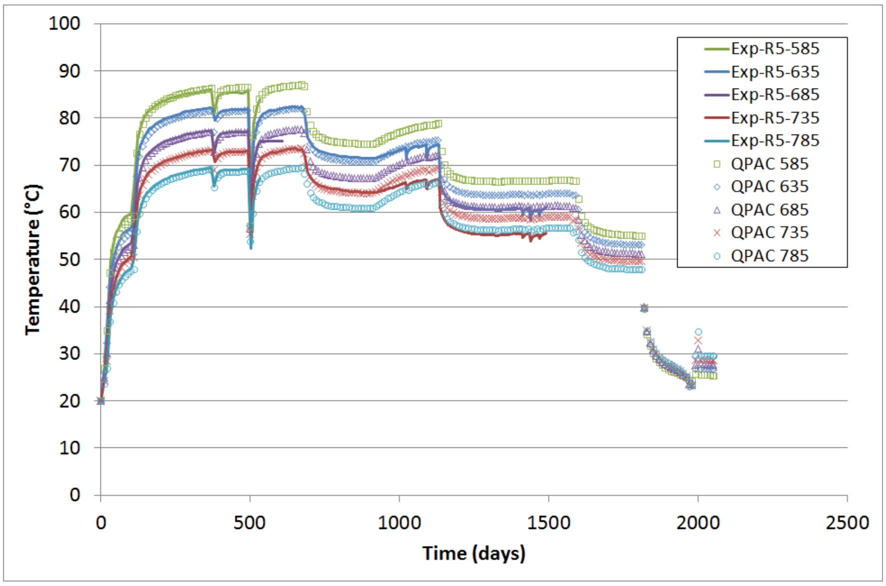

Figure 21: The temperature evolution at 5 locations in the bentonite. Experimental data (solid lines) provided via the THERESA project.

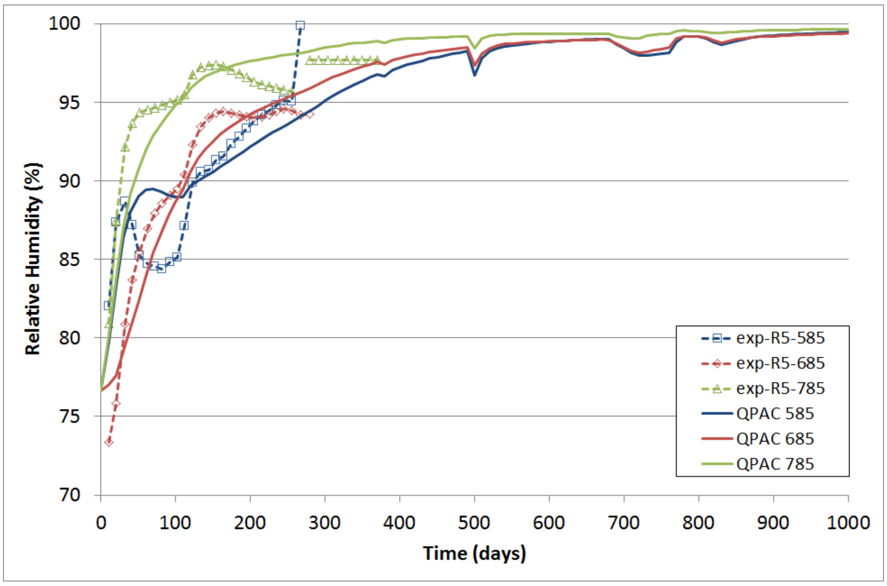

Figure 22: The relative humidity evolution at 3 points in the bentonite. Experimental data (symbols, broken lines) provided via the THERESA project.

6.3.1. Summary of Base Case Comparison

In the comparison performed here, results from several SKB models have been used: 'CRT 1', 'CRT 3', 'CRT 4', 'CRT 6b' and 'THM CRT' (which is the model used in SKB's resaturation study, and may be the same as one of the preceding models). The SKB model providing to best fit to the different CRT measurements varies according to the measurement data being considered. The QPAC results are from a single model, and hence it is unlikely that the fit to the data will be quite as good as the SKB models in all cases.

Nevertheless a reasonable level of agreement has been demonstrated between the SKB models and the QPAC model when applied to the CRT test. Both models provide an acceptable fit to the CRT data, with the possible exception of the measured angular stress, although as noted in TR-10-11 there is reason to suspect that the measurements may not be truly representative of compacted bentonite due to the application of bentonite powder around the sensors. In particular both models provide a very good fit to the final homogenised void ratio at the end of the experiment and the suction (although some of the SKB models provide a relatively poor fit to the measured data closest to the canister). The timescales for resaturation in the QPAC model and the 'THM CRT' model also agree very closely, although no measured CRT data appears to have been presented by SKB that would allow these predictions to be related back to the measurements. This is discussed further in Section 6.5.

The intercomparison results suggest that there is good reason to suspect that any observations and 'lessons learned' with the QPAC model may also be relevant to the SKB model.

6.4. Sensitivity Studies

6.4.1. Intrinsic Permeability

The intrinsic permeability used in the QPAC model is a function of the open porosity, θ, and is given by the expression

$$
\begin{aligned}
k(\theta) &= A(\theta)k_0 \\
A(\theta) &= 2.5\times10^{10(\theta-0.2)}
\end{aligned}
$$

where $k_0 = 10^{-22}$ m^2. This expression was derived from data supplied to the THERESA project (THERESA, 2008). The formulation used here is different to that used in SKB's THM models, which is based on the Kozeny-Carman equation, and is also different to that used in SKB's TH models, which assume a fixed intrinsic permeability (because porosity variation is not included in the TH models). Values for the reference permeability are given in Table 6; two variant cases are considered, one with a value a factor of 10 larger than the base case, and one with a value a factor of 10 smaller than the base case. The reference block permeability assumed in SKB's THM models is 1.09-2.18×10^{-21} m^2, therefore Case 1 presented here gives a closer fit to SKB's permeability model.

Table 6: Values of the reference permeability used in the modelling

Case	Reference Permeability k_0 (m^2)
Base	1e-22
Case 1	1e-21
Case 2	1e-23

Changing the intrinsic permeability of the bentonite by an order of magnitude in each direction has quite a big impact on the results. A comparison of the axial stresses for each of the three cases is shown in Figure 23. Reducing the permeability greatly reduces the stresses, and, since the water cannot ingress so easily into the bentonite, stresses are smaller nearer to the canister (unlike the other cases where stresses near the canister become larger than those further away after a period of time).

Figure 23: The axial stress evolution at 3 different points in the bentonite, shown for the base case (solid lines) and cases with 10 times larger (dashed lines; Case 1) and smaller (dotted lines; Case 2) intrinsic permeability.

Although some model outputs such as the stresses demonstrate large sensitivity to the intrinsic permeability, others such as the homogenised void ratio do not, as shown in Figure 24. There is very little difference between the base case and Case 1 (10 times larger intrinsic permeability), because full saturation is achieved anyway in the base case; but with 10 times smaller permeability, Case 2, the void ratio is less uniform through the bentonite ring, because the blocks have not completely resaturated by the end of the simulation (2052 days, which is consistent with the duration of the CRT experiment), and is much higher in the pellet region.

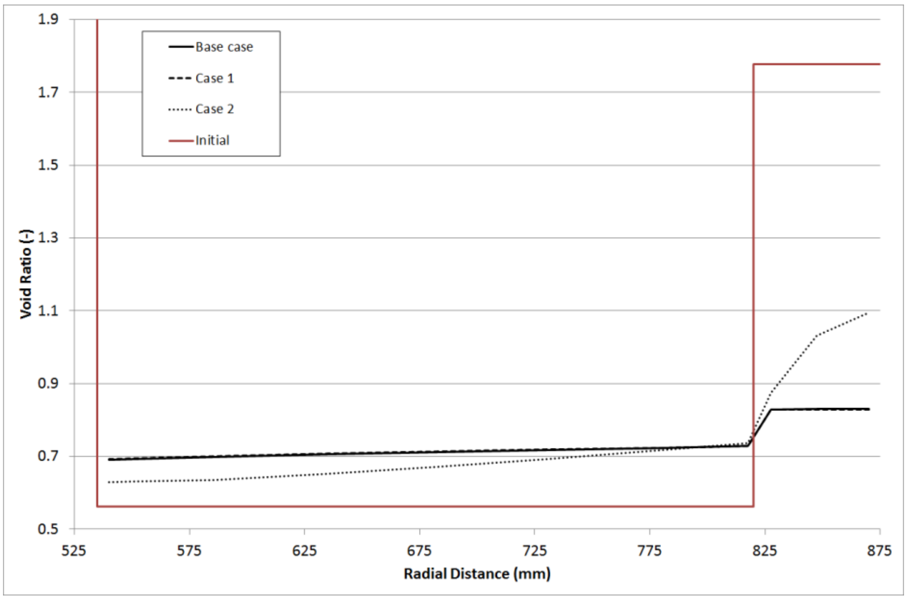

Figure 24: The void ratio profile through the bentonite at the end of the simulation, shown for the base case (solid line) and cases with 10 times larger (dashed lines; Case 1) and smaller (dotted lines; Case 2) intrinsic permeability.

The suction evolution also varies quite considerably between the cases, as might be expected given the rate at which the bentonite can become saturated depending on its permeability. Plots of the suction at 585 mm, 685 mm and 785 mm are shown in Figure 25 for each of the cases. Case 2, with the lower permeability, maintains suction of up to 20 MPa through the simulation because the blocks do not fully saturate in this case.

Both the water ratio and water saturation show similar sensitivity to the permeability as the void ratio, as shown in Figure 26 and Figure 27. As expected, the case with higher permeability (Case 1) is totally saturated by the end of the simulation; whilst the case with lower permeability (Case 2) does not become totally saturated, particularly near the canister.

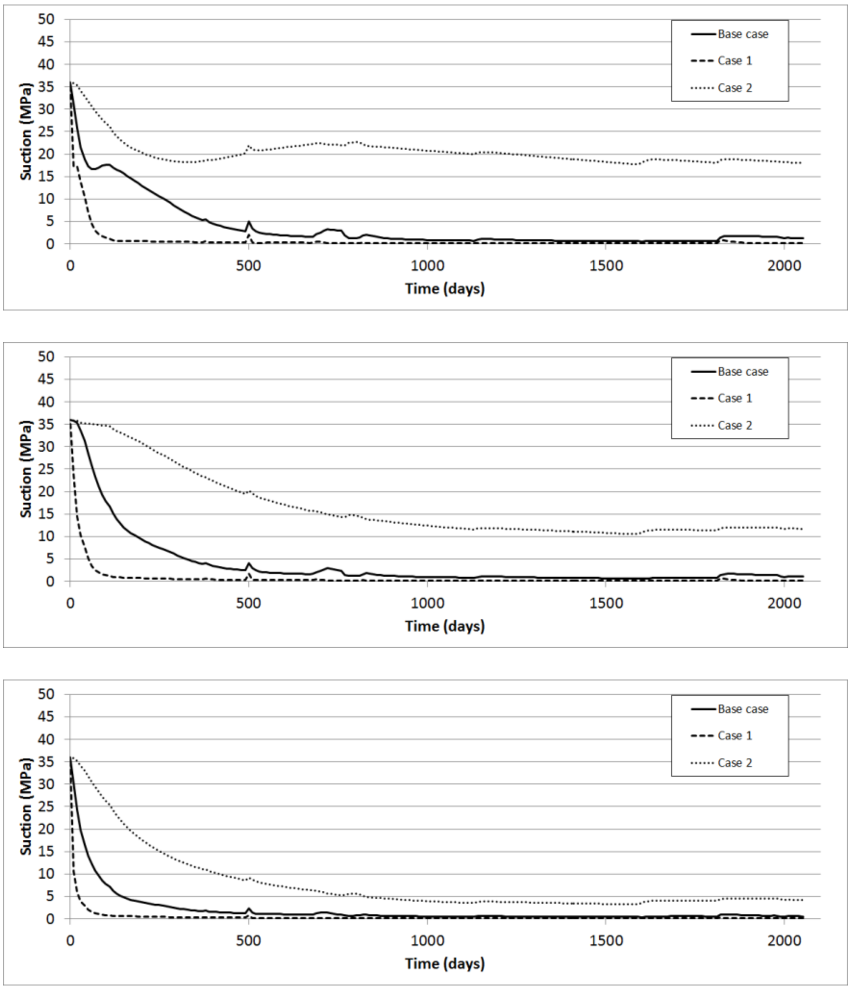

Figure 25: The suction pressure evolution at 3 points in the bentonite; 585 mm (top), 685 mm (middle) and 785 (bottom), shown for the base case (solid line) and cases with 10 times larger (dashed lines; Case 1) and smaller (dotted lines; Case 2) intrinsic permeability.

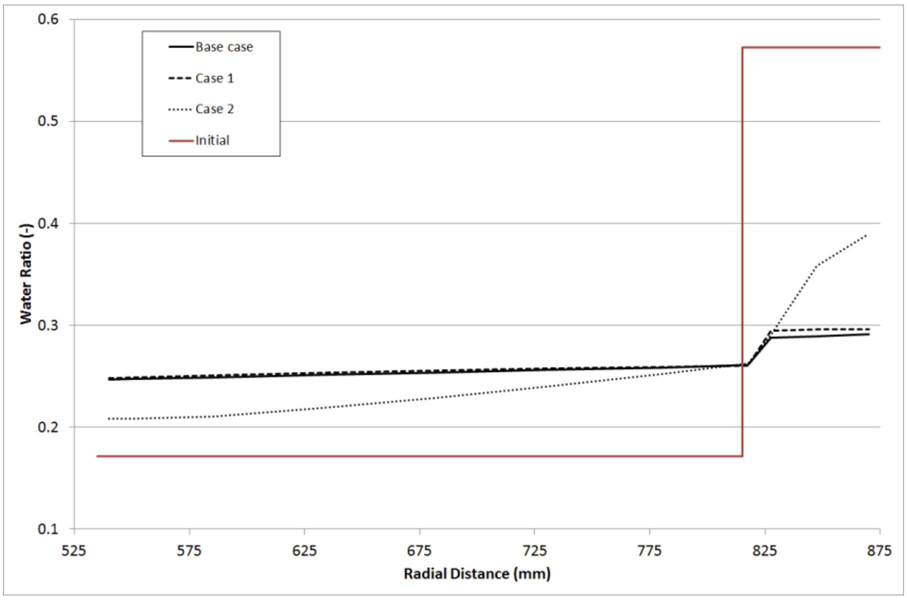

Figure 26: Profile of the water ratio at the end of the simulation, shown for the base case (solid line) and cases with 10 times smaller (dotted line) and larger (dashed line) intrinsic permeability.

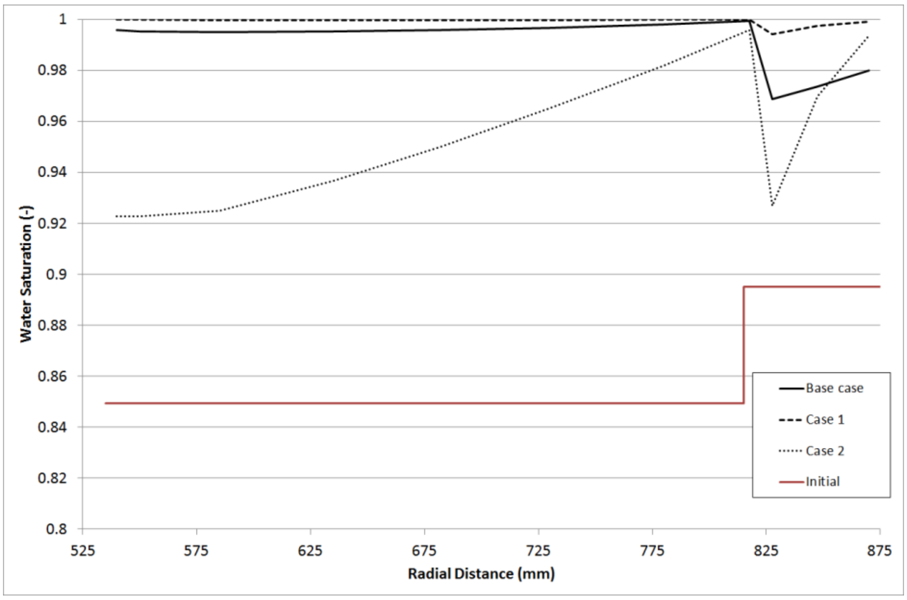

Figure 27: Profile of the water saturation at the end of the simulation, shown for the base case (solid line) and cases with 10 times smaller (dotted line) and larger (dashed line) intrinsic permeability.

6.4.2. Young’s Modulus

Variant cases were considered in which the base case Young’s modulus value, which is taken from TR-00-14 (with some calibration), were multiplied by a factor of 0.5 and 2. Full details are given in Table 7. Note that the value for the pellets is the initial value used in the model; as the pellets swell and become more like the solid bentonite, the Young’s modulus is increased towards the value for the ring.

Table 7: Values of the Young’s modulus used in the modelling

Case	Young’s Modulus (MPa)	
	Ring	Pellets
Base	150	1.5
Case 3	300	3.0
Case 4	75	0.75

The effect on the axial stresses is shown in Figure 28. Stresses are increased initially for the case with the larger Young’s modulus (Case 3) but in the latter stages of the simulation they are decreased by about 10%. Similarly the stresses are initially decreased for the case with the smaller Young’s modulus (Case 4) but then become increased by about 20%.

Figure 28: Evolution of the axial stresses at 3 points in the bentonite, for the base case (solid lines), a case with a Youngs modulus twice as large (Case 3; broken lines), and a case with a Youngs modulus half as large (Case 4; dotted lines).

The impact on the void ratio is quite large for Case 3 (larger Young’s modulus), as shown in Figure 29. The extra stiffness of the bentonite means that it is harder for the pellets to swell and fill the void spaces. Meanwhile, in the ring, the void ratio does not increase as much as for the base case. The reverse effect is seen in the case with the smaller Young's modulus (Case 4), though the impact is not as large.

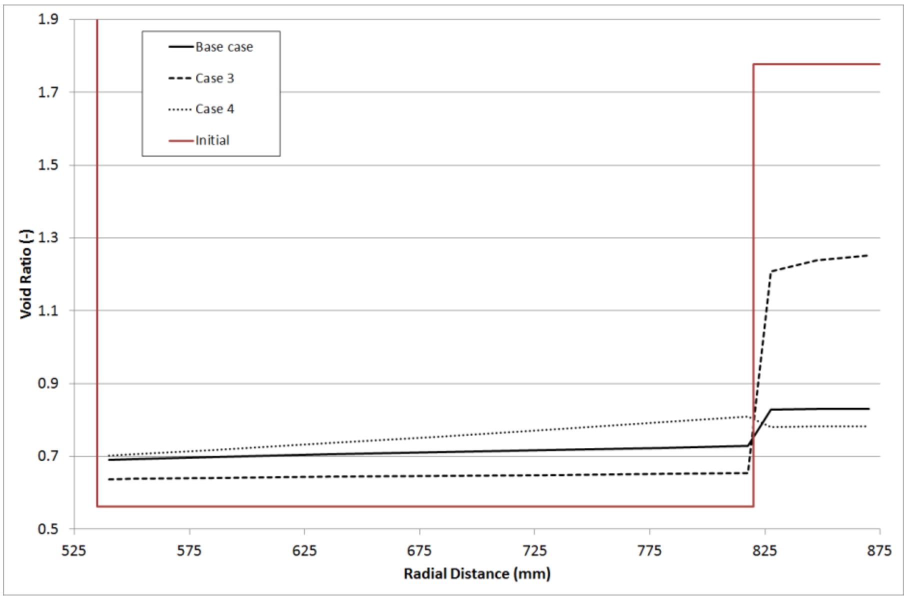

Figure 29: Profile of the void ratio through the bentonite at the end of the simulation, for the base case (solid line), a case with a Youngs modulus twice as large (Case 3; broken line), and a case with a Youngs modulus half as large (Case 4; dotted line).

An effect can also be seen in the suction pressure of the bentonite, shown in Figure 30 for different radial distances. At all points, the suction is higher for the case with the smaller Young's modulus (Case 4) and lower for the case with the larger value (Case 3). It could be argued that Case 3 at least is consistent with the experimental data (shown in Figure 14), despite the fact that the void ratio results for this case are much higher than those measured. However it could also be argued that Case 4 better captures the general rise in the measured void ratios in the outer regions of the blocks approaching the bentonite pellets.

In a similar manner, the water ratio results (Figure 31) show a large deviation in the pellets for Case 3 (larger Young's modulus), but the water saturations (shown in Figure 32) vary only slightly from the base case.

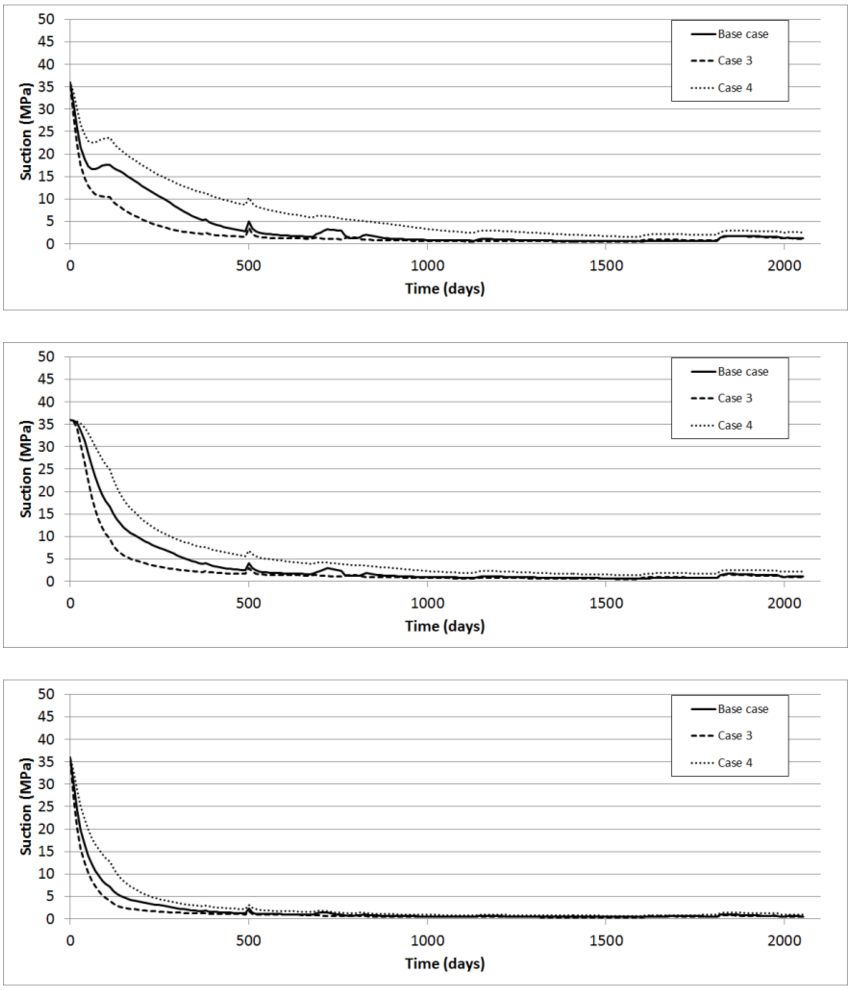

Figure 30: The suction pressure evolution at 3 points in the bentonite; 585 mm (top), 685 mm (middle) and 785 (bottom), shown for the base case (solid lines), a case with a Youngs modulus twice as large (Case 3; broken lines), and a case with a Youngs modulus half as large (Case 4; dotted lines).

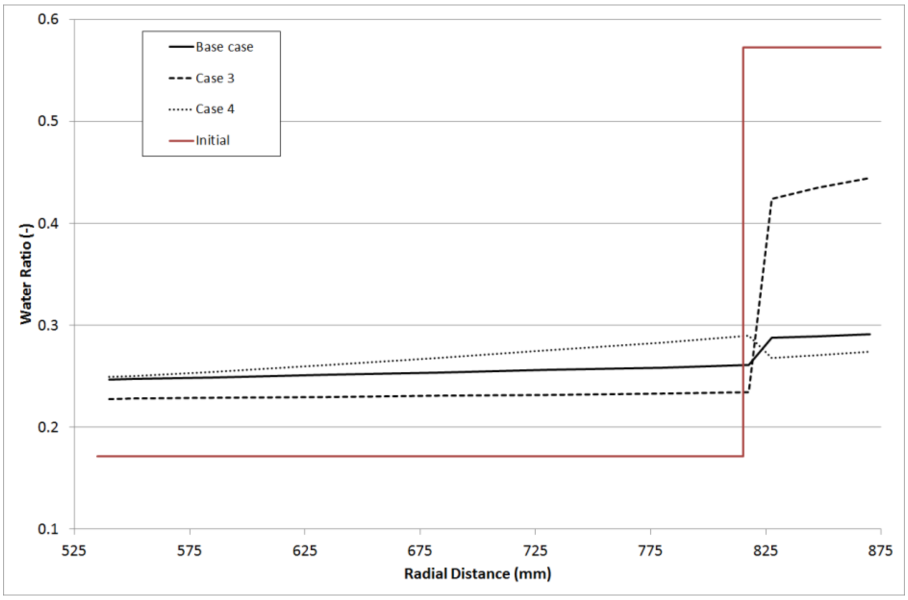

Figure 31: Profile of the water ratio through the bentonite at the end of the simulation, for the base case (solid line), a case with a Youngs modulus twice as large (Case 3; broken line), and a case with a Youngs modulus half as large (Case 4; dotted line).

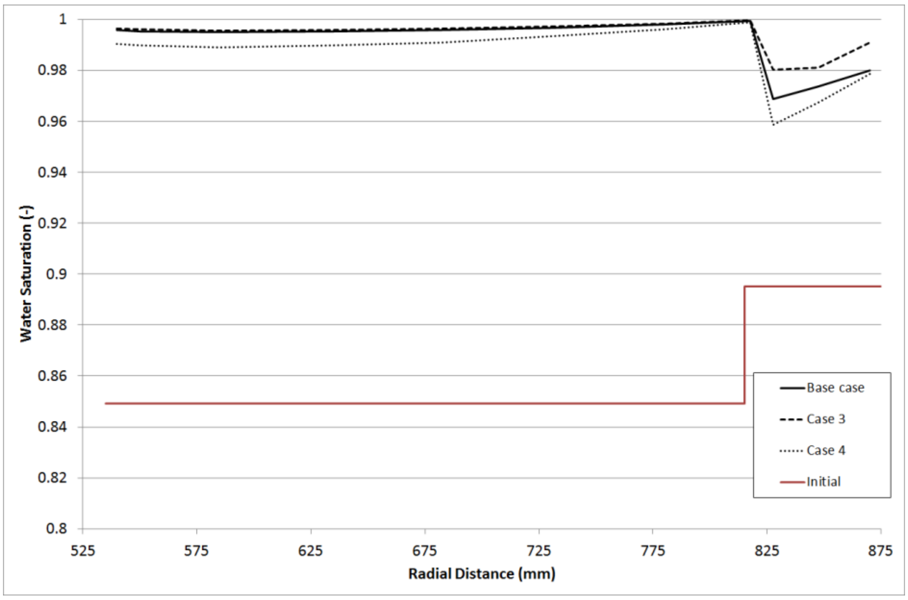

Figure 32: Profile of the water saturation through the bentonite at the end of the simulation, for the base case (solid line), a case with a Youngs modulus twice as large (Case 3; broken line), and a case with a Youngs modulus half as large (Case 4; dotted line).

6.4.3. Vapour Diffusivity

Two variants were considered that used vapour diffusivity values increased and decreased by an order of magnitude from the base case value (from Claesson and Sällfors (2005)). Full details are given in Table 8.

Table 8: Values of the vapour diffusivity used in the modelling

Case	Diffusion Coefficient ($m^2 s^{-1}$)
Base	2.5e-6
Case 5	2.5e-5
Case 6	2.5e-7

The evolution of the relative humidity at 3 different points in the bentonite is shown in Figure 33 for each of the variant cases and the base case. The case with a smaller diffusion coefficient (Case 6) does not vary greatly from the base case, but the case with a larger diffusion coefficient (Case 5) differs in the inner-most regions of the buffer with lower relative humidities during the middle of the simulation as water vapour is carried more rapidly away from the canister. At the start and end of the simulation all three cases give similar results.

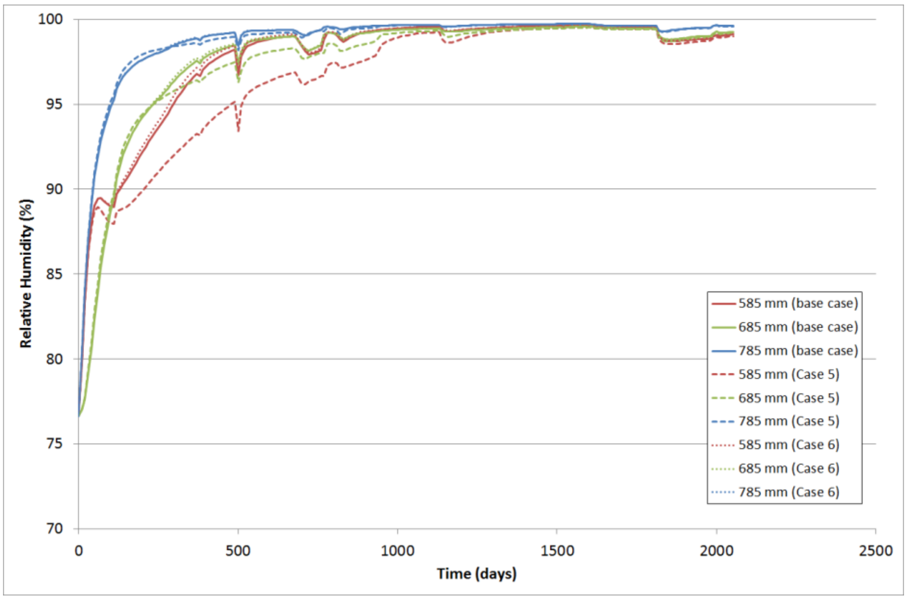

Figure 33: Evolution of the relative humidity at 3 points in the bentonite, shown for the base case (solid lines), a case with an order of magnitude larger vapour diffusion coefficient (Case 5, dashed lines) and a case with an order of magnitude smaller vapour diffusion coefficient (Case 6, dotted lines).

The effect of varying the diffusion coefficient for vapour on other model outputs such as the axial stresses (Figure 34) and suction pressure (Figure 35) is minimal.

The void ratio, water ratio and water saturation are almost identical for the three cases (and hence are not shown).

Figure 34: Evolution of the axial stress at 3 points in the bentonite, shown for the base case (solid lines), a case with an order of magnitude larger vapour diffusion coefficient (Case 5, dashed lines) and a case with an order of magnitude smaller vapour diffusion coefficient (Case 6, dotted lines).

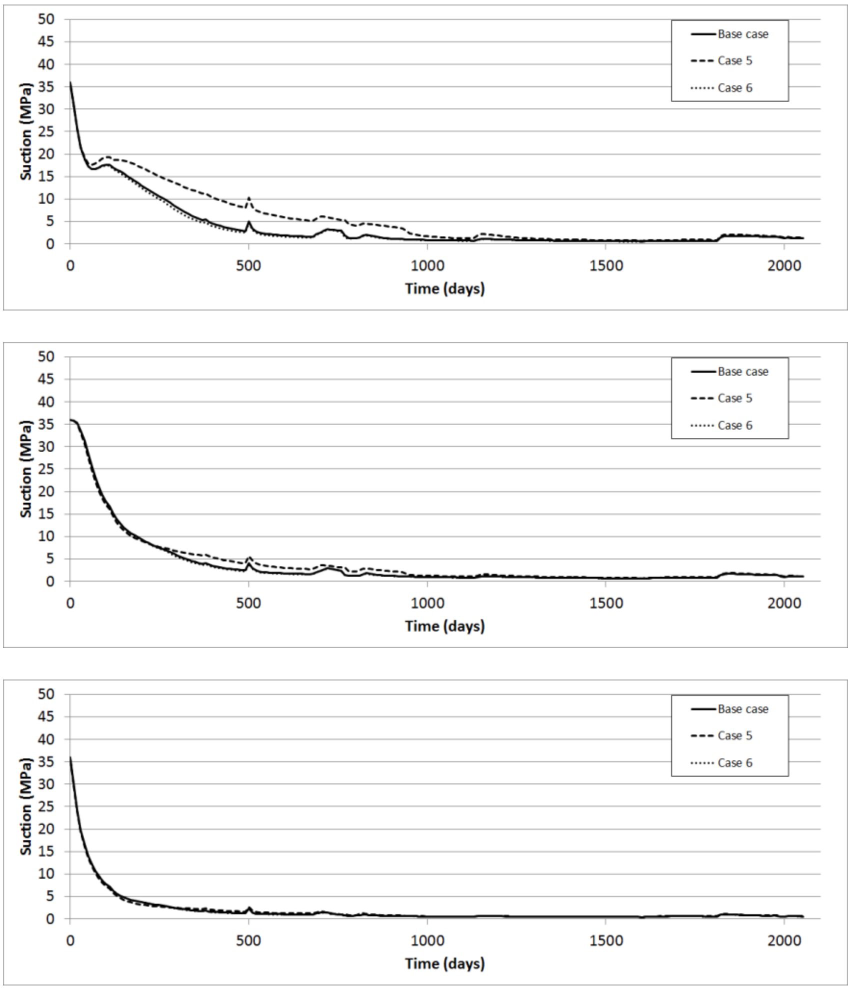

Figure 35: The suction pressure evolution at 3 points in the bentonite; 585 mm (top), 685 mm (middle) and 785 (bottom), shown for the base case (solid lines), a case with a vapour diffusion coefficient an order of magnitude larger (Case 5; dashed lines), and a case with a vapour diffusion coefficient an order of magnitude smaller (Case 6; dotted lines).

6.4.4. Initial Porosity

The sensitivity to the initial emplaced bentonite porosity was tested using two variant cases where the initial porosities in the ring and pellets were 110% and 90% of the base case value, as shown in Table 9. Whilst the initial porosities are given as part of the CRT specification (e.g. THERESA, 2008) and are unlikely to be subject to much uncertainty, these variant cases serve to further demonstrate the sensitivity of the system to small changes in input parameters. The case in which porosity is reduced may also provide useful information that might be relevant if only a fraction of the pore space is available for transport.

Table 9: Values of the initial bentonite porosity used in the modelling.

Case	Initial Porosity (-)	
	Ring	Pellets
Base	0.36	0.64
Case 7	0.396	0.704
Case 8	0.324	0.576

The effect on the axial stresses is shown in Figure 36, and is quite large. The case with the larger porosities results in stresses approximately half of those generated by the base case, whilst the case with smaller porosities results in stresses over twice as large. It is perhaps worth noting that the stresses produced by the model with the larger porosity are more consistent with the measured data (Figure 12) although, as noted earlier, there is some uncertainty regarding the accuracy of these measurements (the results are consistent with the idea that the region around the probes had a 'locally larger porosity').

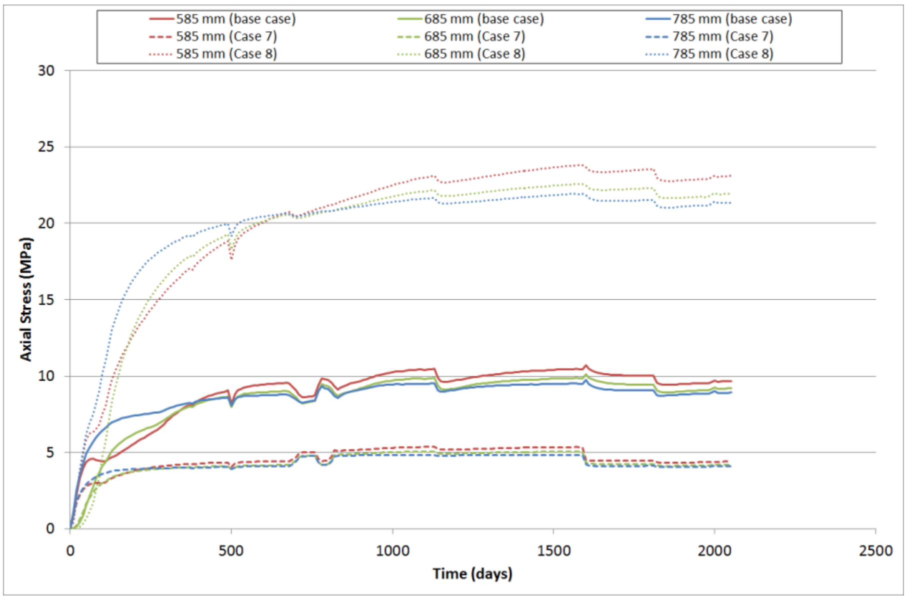

Figure 36: Evolution of the axial stress at 3 points in the bentonite, shown for the base case (solid lines), a case with initial porosities 110% of the base case value (Case 7, dashed lines) and a case with initial porosities 90% of the base case value (Case 8, dotted lines).

The void ratio profile, shown in Figure 37, also differs greatly between the cases. For the case with the larger initial porosity (Case 7) the void ratio in the pellets is barely reduced from its starting point whilst that of the ring is slightly larger than the base case. The results from the case with the smaller initial porosity (Case 8) are closer to the base case results, but show smaller void ratios in both the ring and the pellets.

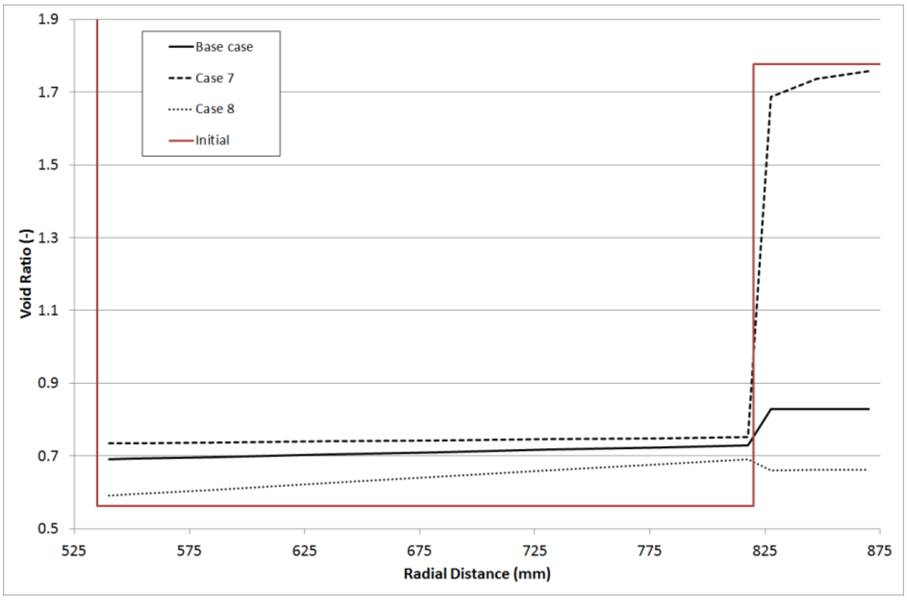

Figure 37: The void ratio profile through the bentonite at the end of the simulation, shown for the base case (solid line) and cases with initial porosities 110% of the base case value (dashed lines; Case 7) and 90% of the base case value (dotted lines; Case 8).

The porosity affects the suction pressure, as demonstrated by Figure 38 which shows the suction at 3 different points in the bentonite. At each location the case with the larger porosity (Case 7) has a smaller suction than the base case, and the case with the smaller porosity (Case 8) has a larger suction, which reflects the faster and slower rates of resaturation in each case respectively.

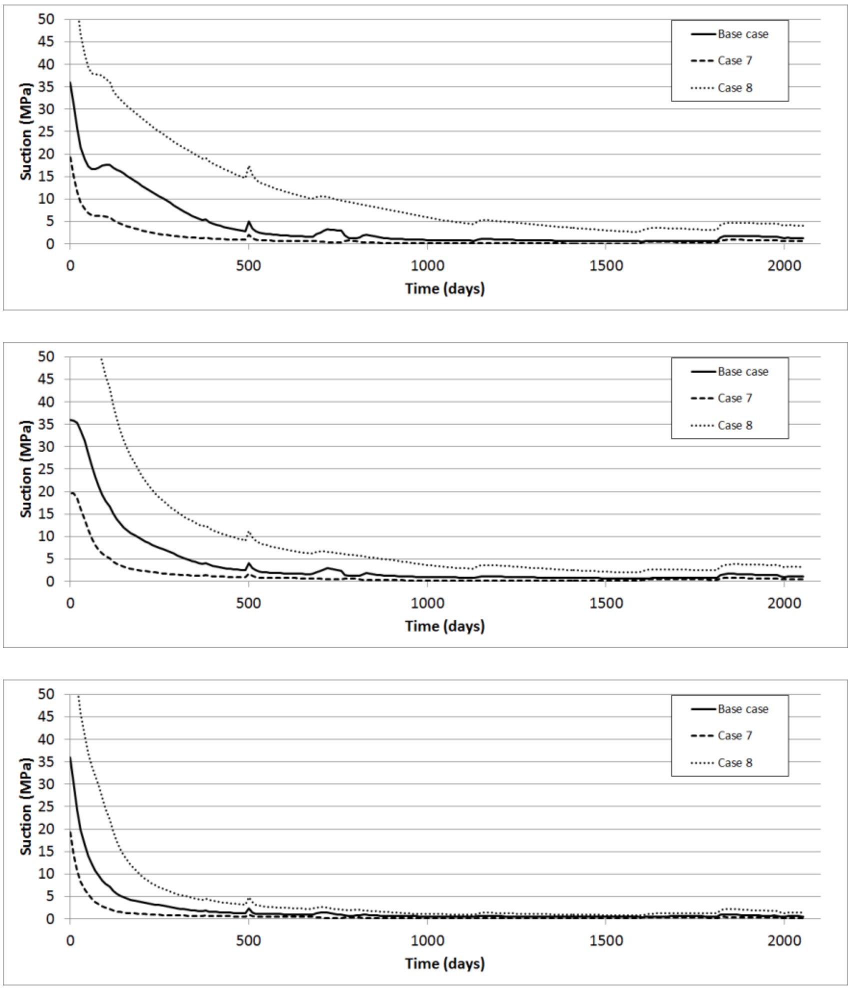

Figure 38: The suction pressure evolution at 3 points in the bentonite; 585 mm (top), 685 mm (middle) and 785 (bottom), shown for the base case (solid line) and cases with initial porosities 110% of the base case value (dashed lines; Case 7) and 90% of the base case value (dotted lines; Case 8).

The water ratio profile (Figure 39) for these variant cases is similar to the void ratio profile, with the water ratio in the pellets for Case 7 (larger initial porosity) ending up higher than the initial value. The impact on the water saturation (Figure 40) is less dramatic, with similar results in the bentonite ring but differing values in the pellet region.

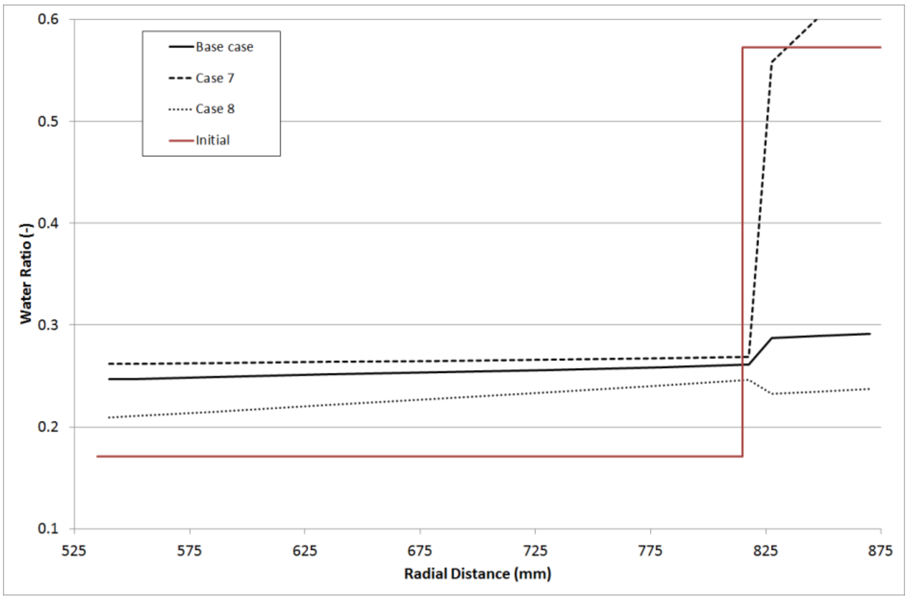

Figure 39: Profile of the water ratio at the end of the simulation, shown for the base case (solid line) and cases with initial porosities 110% of the base case value (dashed line; Case 7) and 90% of the base case value (dotted line; Case 8).

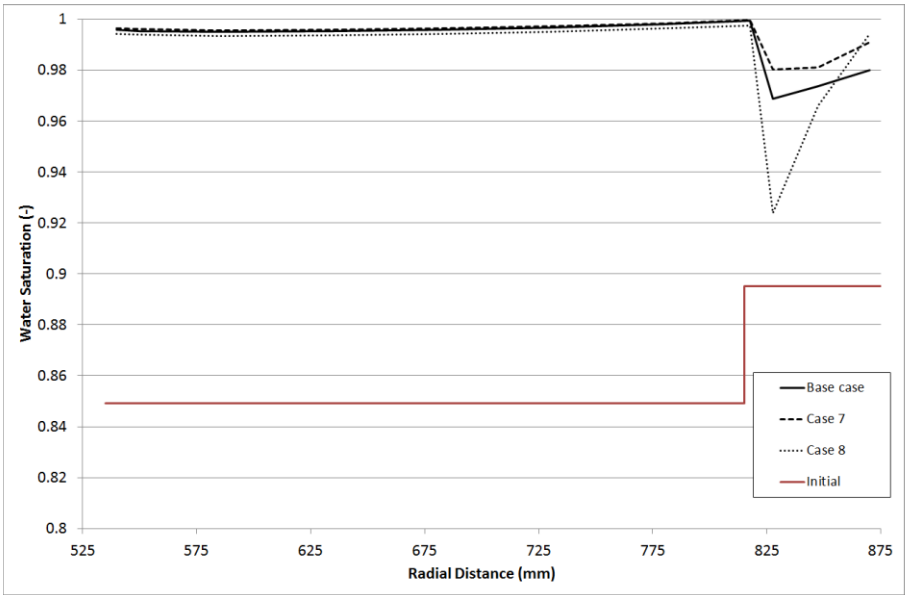

Figure 40: Profile of the water saturation at the end of the simulation, shown for the base case (solid line) and cases with initial porosities 110% of the base case value (dashed line; Case 7) and 90% of the base case value (dotted line; Case 8).

6.4.5. Summary of Variant Cases

Varying the intrinsic permeability has the obvious effect of slowing or increasing the rate of resaturation in the bentonite, with complete saturation not occurring by the end of the simulation at 2052 days for the case in which the permeability was reduced by an order of magnitude. A saturation of 0.95 was obtained at the middle location in the blocks (685 mm) in ~200 days in the base case (Figure 17), and was achieved by around ~2000 days when the permeability was reduced by an order of magnitude. Therefore, in the model, the rate of resaturation varies approximately linearly with the permeability as might be expected from the way in which it is parameterised.

The effects of this on the evolution of quantities in the system that are directly related to the degree of saturation, such as the suction, are fairly obvious. Suction pressures remain high for the entire simulation when the permeability is reduced since complete resaturation does not occur. Similarly stresses are largest away from the canister for the simulated period when the permeability is reduced, but this is likely to reverse as the saturation front progresses.

Decreasing the Young’s modulus reduces the stiffness of the bentonite and allows it to deform more easily. This slows the progress of the resaturation front and so, to some extent, the response of the system to the reduced Young’s modulus is similar to the case in which the permeability is reduced (although the variation from the base case is less marked than the perturbed permeability case presented in 6.4.1 where the permeability was decreased by an order of magnitude). Properties related to the saturation, such as suction, respond accordingly.

The effect on the homogenised void ratio in the blocks is as expected, with the increased Young’s modulus causing less deformation and hence the void ratio remains closer to its emplaced value than the base case.

The good agreement between the measured and computed void ratios in the base case (Figure 13), and the difference to the void ratio introduced by the perturbation to the Young’s modulus, is perhaps good evidence to suggest that the Young’s modulus value is consistent with the observations. However the gradual rise in the void ratio that is seen in the measured data for block regions approaching the pellets is perhaps better reflected in the computed void ratios when the Young’s modulus is halved.

Varying the vapour diffusivity only has a significant effect on the relative humidity, with the coupling to the other quantities in the model being minimal. The reasonable agreement between the base case and the measured values (Figure 22) would tend to suggest that the base diffusivity value is consistent with observations.

Varying the initial porosity had a large effect on the computed axial stresses and on the transient suction behaviour due to the affect that the modified porosity has on the rates of resaturation. The longer term homogenised void and water ratios in the buffer were unaffected, but the corresponding ratios in the pellets varied greatly.

The general conclusion from the variant cases would seem to be that there are some properties in the model, such as vapour diffusivity, that have little feedback on the wider behaviour in the system. Some properties, such as the Young’s modulus would appear to provide a control that can better match some aspects of the measured data (in this case the homogenised void ratio).

The variations that most greatly affect the computed behaviour in the model were the perturbations to the intrinsic permeability and the initial porosity. These produced a greater difference in many of the outputs of the model that could mostly be explained by the fact that these changes modified the underlying rate of change of resaturation of the bentonite. Some of the differences caused by these perturbations are only relevant to the transient period while the bentonite is resaturating, and are not seen in the final homogenised state (e.g. effects on void ratio) while other quantities such as the homogenised axial stress are fundamentally affected.

The results suggest that an accurate prediction of the rate of resaturation of the bentonite is a critical factor in producing reliable predictions for the wider behaviour of the buffer, affecting not only the transient period during resaturation, but also affecting the homogenised state when resaturation is complete. SKB acknowledge that the timescales of resaturation in the CRT test are fast and state that (TR-11-01, Page 372):

"The relation between the saturation responses for TH-models and Thermo-Hydro-Mechanical (THM)-models has only been investigated for rapid saturation processes".

For situations in which the supply of water might lead to slower rates of resaturation (e.g. when resaturating from a single, low transmissivity fracture) an accurate model of the resaturation will be especially important.

The effect of the water supply on the rates of resaturation in the model are investigated in the following section.

6.5. Effect of the Water Pressure Boundary Condition

In the CRT experiment, a time-varying water pressure boundary condition was applied to the buffer using filter mats installed on the rock surface. The configuration of the mats is as shown in Figure 41. Each filter mat was 10 cm wide, with length stretching from the bottom of the deposition hole to the bottom of the top-most bentonite ring (so 0.75 m shorter than the deposition hole depth). 16 mats were used (if the figure is accurate) resulting in a 'water supply coverage' of the buffer surface of around 26%. Assuming that the water supply from the filters remained available to the bentonite for the duration of the experiment, these boundary conditions would seem to equate to a high net rock transmissivity. The measured hydraulic conductivity of the filter mats is around 10^{-4} m/s (Börgesson, 2007).

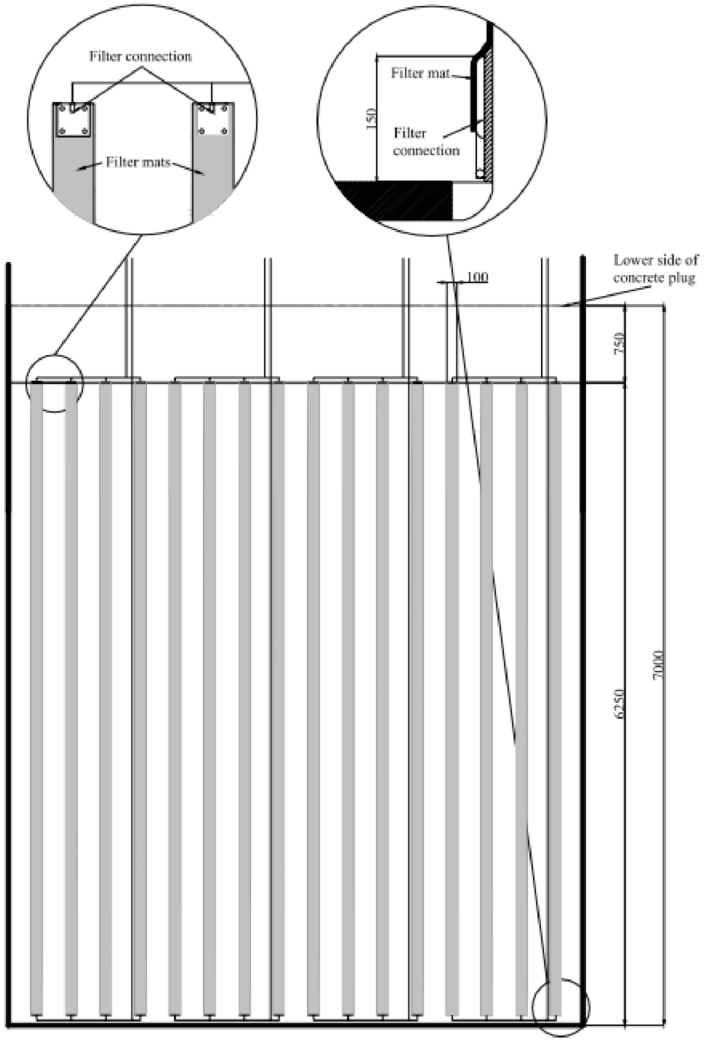

Figure 41 Schematic drawing of the location of the filter strips and connecting tubes in the wetting system. The surface of the deposition hole has been unfolded (Reproduction of Börgesson, 2007, Figure 8)

The water pressure that was imposed in the experiment varied according to the schedule given in Table 10. The water pressure boundary condition in the base case model replicates this.

To investigate the effect of variations in supply of water on the rates of resaturation predicted by the model, three variant cases were run with fixed pressure boundary conditions of varying magnitudes, as shown in Table 11.

Table 10 Imposed Boundary Water Pressure in the CRT

Day	Applied Water Pressure (MPa)
0	0
714	0.8
770	0.1
805	0.4
819	0.8
1598	0
1877	0

Table 11: Rock pressure boundary conditions used in the modelling.

Case	**Rock Boundary Pressure (MPa)**
Base	Time-varying
Case 9	0
Case 10	0.01
Case 11	0.1

The water saturation evolution from each of the variant cases is shown in Figure 42 (pellets), Figure 43 (mid-ring) and Figure 44 (near canister). The corresponding saturations from the base case, in which the time-dependent boundary condition is applied, are also shown. The only appreciable differences between the four curves are in the pellet region, where there saturation rapidly rises above 96% for all of the cases that were considered.

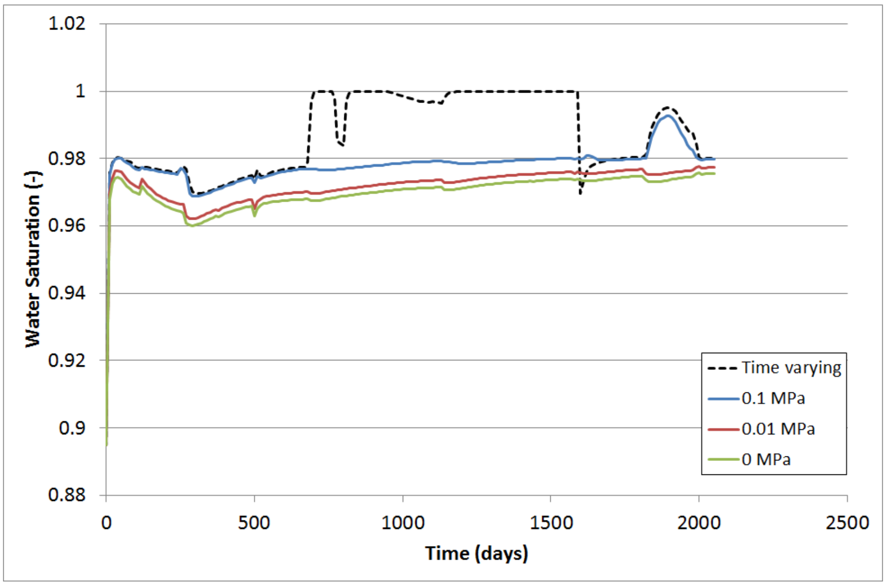

Figure 42: Evolution of water saturation in the pellet region for 3 fixed-pressure boundary conditions and the base case (broken line).

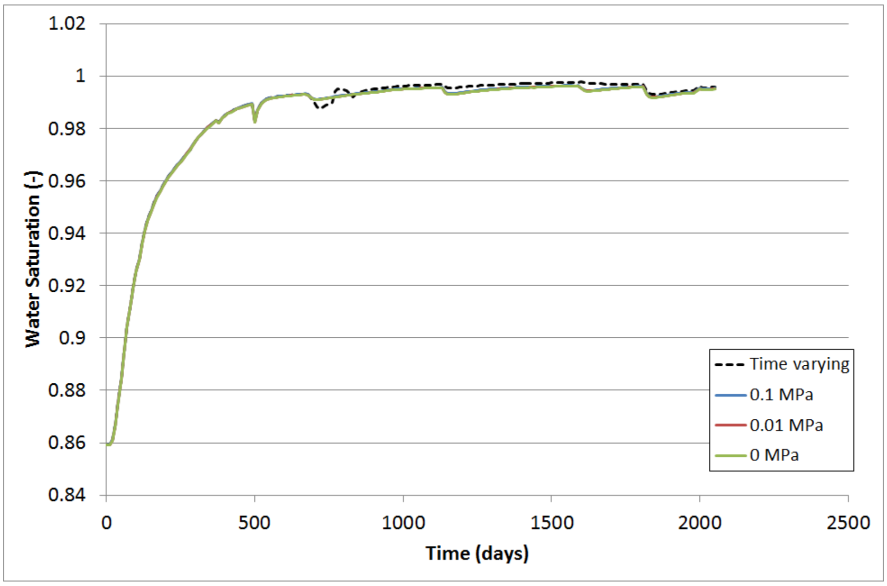

Figure 43: Evolution of water saturation at the mid-point of the bentonite ring, for 3 fixed-pressure boundary conditions and the base case (broken line).

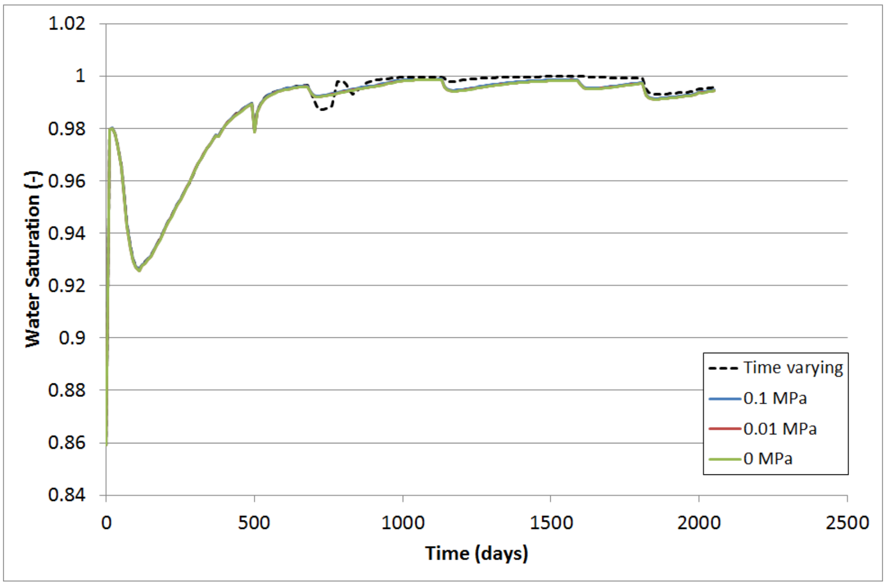

Figure 44: Evolution of water saturation in the bentonite ring near the canister, for cases with fixed-pressure boundary conditions and the base case (broken line).

The predicted rates of resaturation in the model are seemingly insensitive to the applied water pressure at the boundary. This is not necessarily surprising. The way that the model is configured is for the bentonite suction to provide the driving force for the flow, with the only resistance to flow occurring due to reductions in water saturation via the relative permeability (although since saturations are generally increasing the relative permeability will not decrease) or reductions in porosity via the intrinsic permeability formulation (as described in Table 5). SKB’s THM models are similarly configured, albeit with mildly different functional dependence on saturation and porosity and SKB’s TH models are only configured to reduce permeabilities in response to decreases in saturation (since the porosity is fixed in the TH models). Therefore it is possible that both SKB’s TH and THM models will be similarly indifferent to the change in boundary conditions.

The overall mass balance in the system can be inferred from the cumulative water inflow from the rock boundary into the buffer. This is shown in Figure 45. As expected from the water saturation results, there is little difference in the calculated inflow between the cases that have been considered, even for the case in which a zero pressure is applied.

The QPAC 1-D model has a notional height of 10 cm. To estimate the total cumulative water inflow that would be observed if the model was applied to the full deposition hole volume the QPAC results have been scaled. The scaling was performed by multiplying the model inflow by the ratio of the canister height (4.835 m) to the model height (0.1 m) to give an estimate of the total inflow around the canister. A second model was then run by modifying the QPAC model to incorporate a thinner canister (radius 5 cm) with the extra space being filled with bentonite block material, in order to approximate the inflow in the regions above and below the canister. This was then multiplied by the ratio of the bentonite cylinder height (7m – 4.835 m = 2.165 m) to the model height (0.1 m) and added to the previously calculated inflow around the canister. This approach will only provide a crude estimate of the rate of resaturation that would have been seen in an equivalent

2-D model because of the absence of the possibility for upward and downward flows around the canister 'corners' in the combined 1-D models.

The estimated cumulative inflows for the various pressure boundary condition models are plotted with the measured inflow from the CRT experiment (Goudarzi et al., 2006) in Figure 46. The estimated cumulative inflows from each model are very similar due to the similarity in the resaturation patterns. Whilst a good match to the measured data is obtained initially, the measured inflow quickly tails off in the period after ~250 days, whilst the modelled inflow continues at a steady rate. By 600-700 days the measured inflow in the experiment appears to have almost stopped. This suggests that the imbibition process in the experiment became inhibited in a way that is not represented in the QPAC model.

At the time at which the pressure boundary condition was ramped up in the experiment the inflow of water is seen to restart. Again, over time there is a gradual tailing off of the inflow rate although it does not completely stop until the applied pressure on the boundary is removed.

The total amount of water in the system at the end is of a similar magnitude in both the experimental results and the model, although as noted above the upscaling of the 1-D results to provide inflows to the entire deposition hole is crude.

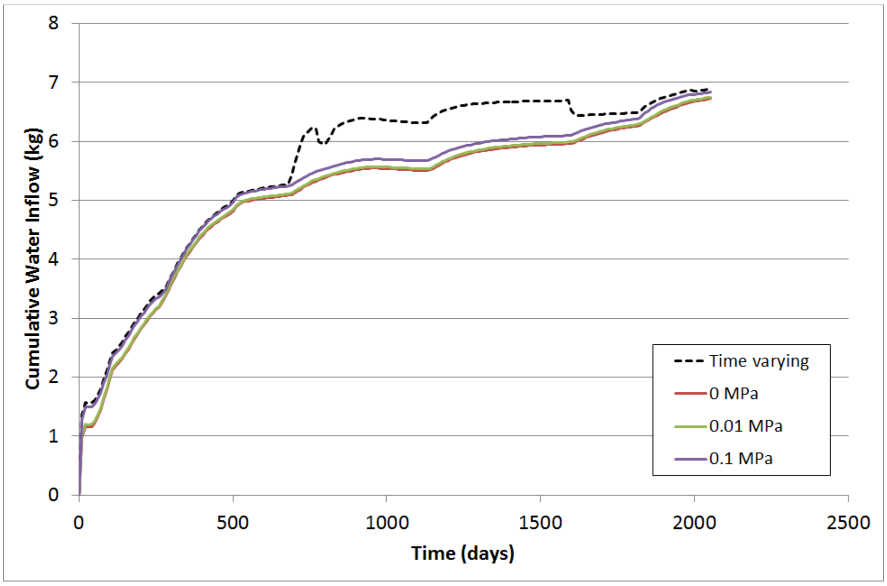

Figure 45: The cumulative water inflow for the 10 cm tall 1-D model, for a variety of fixed-pressure boundary conditions and the time-varying pressure boundary condition base case (broken line).

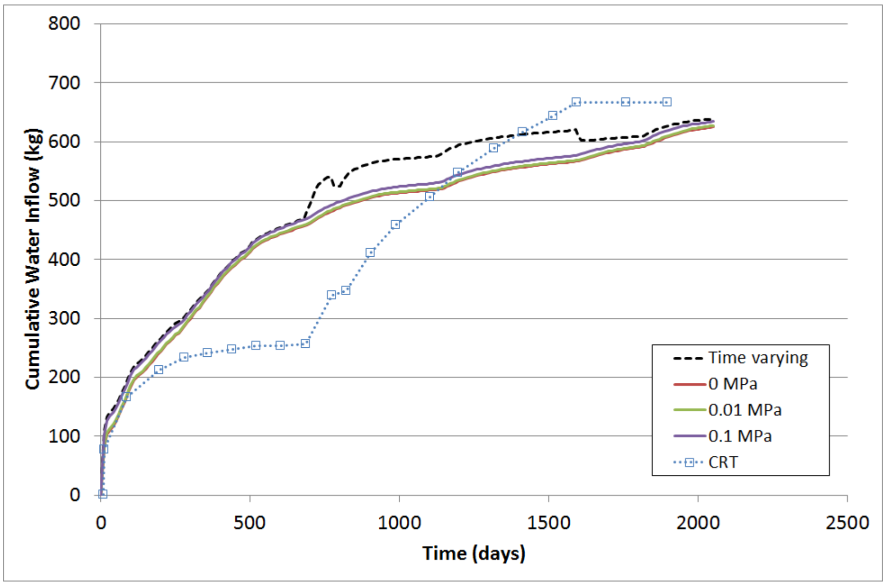

Figure 46: The cumulative water inflow for the whole system, scaled up from the 1-D model. The CRT measurements are from Goudarzi et al. (2006).

6.6. Conclusions

The 1-D QPAC model of the CRT experiment has been shown to behave similarly to the SKB 'THM CRT' model. Both models match the CRT measurements that are considered by SKB in TR-10-11. Due to the similarity in the results of the QPAC and SKB models, and the underlying equations that are implemented in both models, it is expected that both models might respond similarly to perturbations in their input parameters and boundary conditions.

A short study was undertaken to identify parameters that the model outputs may be sensitive to. Of the perturbations that were considered it was found that the parameters that the model outputs were most sensitive to were those that directly impacted upon the rate of resaturation. The parameters that had less effect on the rate of resaturation affected the overall solution less.

The sensitivity of the rate of resaturation to the availability of water was then investigated by varying the applied water pressure on the boundary. The model results, which may be similar to those that would be seen if the same perturbations were applied to the SKB models, were shown to be largely insensitive to this change. This was in contrast to the CRT measured inflow data, which showed a clear response to changes in the applied water pressure in the filter mats. Moreover the CRT data indicated that, even though a largely homogeneous water contact was present, the rates of resaturation appeared to tail off to zero when there was no externally applied pressure. This was presumed to be caused by the development of a resistance to the inflow in the buffer, which was not represented in the models. Increasing the external pressure in the experiment allowed the buffer to begin resaturating again, but the rate of resaturation was seen to reduce with time and might be expected to eventually fall to zero again if the experiment was continued for long enough (and if the buffer did not fully resaturate in that time).

The inability for the models to replicate this seemingly key behaviour, which would control the overall timescales for resaturation, does not lend confidence that the models can be applied to accurately simulate the more likely resaturation patterns that would be expected in and around deposition holes where the water supply is more limited and localised to small fractures.

The CRT data itself raises some questions over the conceptual model describing how resaturation is expected to occur in the buffer. From the point of view of buffer resaturation, the bentonite is required to have the ability to draw water into the deposition hole and distribute it evenly around the buffer until it becomes homogenised. At this point in time the required role of the bentonite changes and it is expected to provide a hydraulic barrier to prevent advection. It is possible that these contrasting required behaviours of the bentonite are leading to the 'self-limiting' behaviour that seems to have been observed in the experiment. Initially, with no applied external pressure the suction exerted by the bentonite draws some water into the buffer to saturate the bentonite close to the water supply. As this location fully saturates, the swelling pressure increases and it begins to act as a hydraulic barrier. The suction in the bentonite deeper into the buffer must be sufficient to overcome the hydraulic resistance if the water is to move further into the buffer. Thicker regions of fully saturated bentonite will provide a greater resistance to flow and the fact that the rate of inflow is seen to stop suggests that the suction pressure that is exerted is insufficient to overcome the resistance when a sufficiently 'thick' region of saturated bentonite is present. This is possibly a consequence of the lack of a connected flow porosity in the complicated bentonite pore structure (which suggests that the currently-implemented dependence of permeability on porosity is inappropriate for MX80). When the externally applied pressure is increased this provides an extra force allowing water to move further into the buffer. However the rate of ingress is seen to decrease with time, possibly as a consequence of the development of the hydraulic barrier function in an increasingly thick region of the bentonite.

It is recognised that the pressure boundary conditions that were applied in the Canister Retrieval Test were lower than the natural hydrostatic conditions that could be expected to be present under true repository conditions and that a larger external 'driving force' may be present. However, resaturation from a limited number of small fractures around the deposition hole will mean that this driving force is exerted over a much smaller fraction of the buffer surface than in the CRT and will inevitably increase the distance over which water must travel through the bentonite in order to access more remote regions of buffer. It is unclear how these competing factors will interact.

It is not evident that SKB have investigated the possibility that the contrasting required behaviours of the bentonite could lead to difficulties in resaturating the buffer, but they do acknowledge that "It has not been confirmed from studying THM and TH models that the saturation time for the THM model is bounded by the saturation times for the TH models for slow wetting processes." (TR-10-11, p84).

It is suggested that further work is performed to investigate the likely in-situ behaviour when resaturation occurs from small fractures. Either the possibility of difficulties for resaturation should be dismissed, or the impact on the safety case should be investigated if the hypothesised behaviour is genuinely possible. Evidence from other in-situ experiments do not appear to reproduce the self-limiting behaviour. For example, Figure 47 suggests that the measured water content in the FEBEX in-situ experiment (FEBEX, 2012) continued to increase over the first nine years of the experiment. The FEBEX bentonite is an approximately 1:1 Na:Ca mixture, whereas MX80 is around 4:1, and has a lower montmorillonite content than

MX80 (Cui et al., 2011). Therefore differences in the hydro-mechanical properties of more Ca-rich bentonite must be taken into account when considering the relevance of this experimental data. For example data presented by Cui et al. (2011) suggests that the swelling potential of FEBEX bentonite at a suction of 20 MPa is around 15%, whereas MX80 is closer to 40%. Therefore it would not necessarily be expected that the two bentonites would exhibit similar hydraulic behaviour. The Ibeco bentonite, which is proposed as an alternative bentonite in SR-Site, has a monovalent :divalent cation ratio of around 1:3 and so its hydro-mechanical properties could be quite different to MX-80. However the resaturation/homogenisation modelling in TR-10-11 only considers the MX80 bentonite.

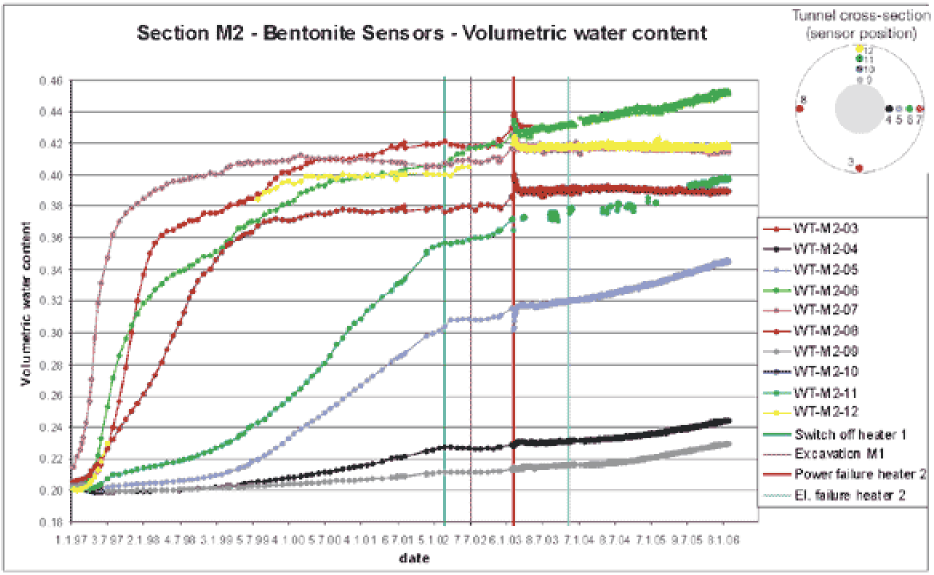

Figure 47 Measured water content in the FEBEX II experiment (from http://www.grimsel.com/gts-phase-v/febex/febex-ii-results-to-date-)

One potential situation that could arise if the hypothesised behaviour is possible is that the buffer could either equilibrate to a heterogeneously saturated state, or a state of transient heterogeneous saturation could exist for an extended period of the overall evolution of the EBS. If resaturation is from a small fracture adjacent to the canister it may be possible to fully saturate a pathway through the buffer over the relatively short distance to the canister surface before the hydraulic barrier properties of the fully saturated region prevent further water ingress into regions in the buffer that are more distant from the resaturating fracture. This situation is depicted in Figure 4.

6.6.1. Issues and Questions Arising as a Consequence of the Modelling

The primary issue arising from the modelling that has been undertaken is that it would appear that SKB's THM models are not likely to reflect the rates of inflow that have been measured in the well-characterised and constrained CRT test experiment. Models based on fitting this data (which provide a good match to other aspects of the CRT dataset) are used to calibrate the TH models that are used to estimate rates of buffer resaturation that are assumed in the safety case. It is therefore difficult to be confident in the predictions that are made by these models, especially under conditions where the water supply is more limited.

The questions that naturally arise are:

- Are SKB's models similarly insensitive to variations in the water pressure boundary condition?
    - If yes, this would suggest that the rates of resaturation that have been predicted cannot be relied upon.
- Has the 'self-limiting' behaviour that seems to have been exhibited in the CRT data been considered by SKB?
- Is the hypothesised 'self-limiting' behaviour genuine, or is there experimental evidence that might refute it?
- If genuine, how does the self-limiting behaviour affect the wider safety case when in-situ hydraulic conditions are reflected in the models? For example there would seem to be potential for:
    - incoming corrodants to be localised to a fraction of the canister height, thus leading to more focussed corrosion;
    - uneven swelling pressures to develop in the buffer, causing an uneven load on the canister; and
    - sufficiently low swelling pressures to remain in some regions of the buffer which may be insufficient to suppress the activity of microbes (which could still be accessed by diffusing solutes).

  These conditions could exist for an extended period if resaturation is slowed sufficiently, or perhaps persists indefinitely if the self-limiting behaviour is possibly under in-situ conditions.

6.6.2. Issues for Further Investigation

- An attempt should be made to develop conceptual and numerical models that are capable of demonstrating the same response to the externally applied boundary water pressure as seen in the CRT data.
- Once a good fit to the experimental data is obtained (especially the cumulative inflow data), reasoned arguments should be given to suggest why the models should also apply to the more likely resaturation modes in the repository, in particular resaturation from one or more discrete small fractures.
    - New experimental evidence in this area would be extremely valuable.
- The new models should be applied to calculate timescales required for resaturation under repository conditions, particularly those from one or two small intersecting fractures.
- If the timescales for resaturation from the new models are sufficiently longer than those calculated by SKB, the impact on buffer safety functions should be assessed.

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APPENDIX 1

Coverage of SKB Reports

The SKB reports covered in this review are given in Table A1. These include all the mandatory and relevant SKB reports specified in the assignment together with reports that include discussion of the gas release calculations. Additional reports that were identified as containing relevant information and were consulted during the review are listed in Table A2.

Table A1: SKB Reports Reviewed

Reviewed report		Reviewed sections	Comments
No.	Title		
TR-11-01	Main report of the SR-Site project	Summary, 1, 2, 3, 4 (except 4.8) 4.8, 5, 8.3 10.2.4, 10.2.5, 10.3.2, 10.3.8, 10.3.9, 10.3.10, 10.3.12, 10.3.13	Detailed Overview Detailed Detailed Detailed Detailed Detailed
TR-10-11	THM modelling of buffer, backfill and other system components: critical processes and scenarios	2, 3, 5, 6, 7	Detailed. Checking for consistency with other reports on modelling and investigation of underlying experimental evidence. Independent modelling performed.
TR-10-66	Corrosion calculations report for the safety assessment SR-Site.	4.1, 4.2, 4.3, 4.3.1, 4.3.2, 4.3.3, 4.3.5, 5.2.2, 5.2.3, 5.3.1, 5.3.4, 5.3.5	Detailed. Checking of some reported calculations. Additional scoping calculations performed.
TR-10-62	Evaluation of low-pH cement degradation in tunnel plugs and bottom plate systems in the frame of	Summary, 2, 3, 4, 5	Detailed review of summary and Section 5. Brief overview of other sections.

Reviewed report		Reviewed sections	Comments
No.	Title		
	SR-Site		
TR-10-57	SR-Site: Oxygen ingress in the rock at Forsmark during a glacial cycle	Summary, 9	Brief. Used to cross-check review of Section 5.3 of TR-10-66
TR-10-52	Data report for the safety assessment SR-Site	1.1, 5.3, 5.3.5, 5.3.6, 5.3.7, 6.7 and 6.8	Migration properties in buffer, backfill and geosphere. Data affecting radionuclide release (e.g. canister failure times, fuel dissolution rates).
TR-10-51	Model summary report for the safety assessment SR-Site	2.4, 3, 3.2, 3.3, 3.4, 3.18, 3.21, 3.2.4, 5.3.6, 5.3.7	Detailed. Checking for consistency with reports on modelling
TR-10-25	Quantitative modelling of the degradation processes of cement grout	Summary, 2, 3, 4, 5	Detailed review of summary and Section 5. Brief overview of other sections.

Table A2: SKB Reports identified as containing relevant information, which were consulted during the review

Report Number	Report title
TR-06-09	Long-term safety for KBS-3 repositories at Forsmark and Laxemar – a first evaluation. Main report of the SR-Can project.
TR-09-35	Mechanisms and models for bentonite erosion.
TR-10-15	Design, production and initial state of the buffer.
TR-10-16	Design, production and initial state of the backfill and plug in deposition tunnels.
TR-10-25	Quantitative modelling of the degradation processes of cement grout Project CEMMOD.
TR-10-39	SR-Site – sulphide content in the groundwater at Forsmark.
TR-10-42	Mass transfer between waste canister and water seeping in rock fractures: revisiting the Q-equivalent model.

Report Number	Report title
TR-10-57	SR-Site: Oxygen ingress in the rock at Forsmark during a glacial cycle.
TR-10-58	SR-Site – hydrogeochemical evolution of the Forsmark site.
TR-10-62	Evaluation of low-pH cement degradation in tunnel plugs and bottom plate systems in the frame of SR-Site.
TR-10-64	Modelling of erosion of bentonite gel by gel/sol flow.
TR-10-65	Thermo-hydro-geochemical modelling of the bentonite buffer: LOT A2 experiment.
IPR-07-16	Canister Retrieval Test: Dismantling and sampling of the buffer and determination of density and water ratio.

APPENDIX 2

Suggested needs for complementary information from SKB

Areas that have been identified as: requiring further information from SKB; further discussion with SKB; containing gaps in the analysis are provided in the three lists below. The top priority is to clarify understanding of buffer resaturation since this process has a marked impact upon arguments that are made for long-term buffer performance (see in particular Sections 5 and 6).

Questions to SKB

1. Resaturation / Homogenisation:

    a. Are SKB's THM models (TR-10-11, Section 5) capable of reproducing the measured inflow data from the CRT test?

    b. Can more details be provided of the 'THM CRT' model referred to in Section 3 of TR-10-11? Is it the same as one of the models in Section 5?

    c. What is the QA status of the **THM modelling report** TR-10-11? The **Buffer, backfill and closure process report** (TR-10-47, November 2010), which post-dates the THM modelling report (TR-10-11, March 2010) states:

    "*The two main reports referred to in the description of the water saturation phase /Börgesson and Hernelind 1999, Börgesson et al. 2006/ are SKB Technical Reports that have not undergone a documented factual- and quality review. However, they are widely referred to by other scientific groups. The revised model of the wetting phase is included in the buffer THM modelling report /-Åkesson et al. 2010a/, which will undergo a documented factual- and quality review."* (Page 65)

    "*Buffer homogenisation (both natural during the saturation phase and caused by the sealing of erosion damage) and buffer upwards swelling are reported in old SKB Technical Reports but will be updated and reported in a general buffer THM modelling report that will undergo a documented factual- and quality review /-Åkesson et al. 2010a/*." (Page 102)

    Thus it is not clear whether the THM modelling report TR-10-11 has undergone review.

2. How is the q_{zone} flow rate (TR-10-66) calculated/post-processed from SKB's DFN calculations.

3. What is the precise meaning of the deposition inflow criterion of <0.1 L/min (e.g. page 158, para 2 of the main report of the SR-Site project

(TR-11-01)) and how has this criterion been used in the modelling undertaken by SKB?

4. Many of the uncertainties associated with the assessment are inherently unquantifiable, but quantitative estimates of canister failure according to key performance criteria are nevertheless made in a number of instances. For example, the **main** report **of the SR-Site project** (TR-11-01) states that the probability of one canister failing due to shearing during the one million year assessment period is 0.08. However, given that many uncertainties associated with estimating canister failure are not readily quantifiable, how can this statement be justified?

Topics for further discussion with SKB

1. It is recommended that SSM should discuss with SKB the most appropriate way of addressing the QA deficiencies in the documentation supplied to date.

2. It is recommended that SSM should discuss with SKB how best to standardize the format of SKB's future reports of safety assessments and supporting activities. A standardized format should enhance the ability of readers to trace the origins of information and the justifications of the arguments that are made.

3. It is recommended that SSM should discuss with SKB the preparation of a single report of all the data and information that was actually used in the SR-Site assessment. This report should include all the data actually used by SKB when modelling the EBS system and indications of associated uncertainties and references to data sources.

Observed gaps / omissions

1. SKB acknowledge that the TH models used for determining rates of resaturation of the buffer have not been verified for slow resaturation processes with the statement (TR-11-01, Page 372): *"The relation between the saturation responses for TH-models and Thermo-Hydro-Mechanical (THM)-models has only been investigated for rapid saturation processes".*

APPENDIX 3

Suggested review topics for SSM

Areas that have been identified as requiring further review, or further analysis are provided in the two lists below.

Areas requiring further review:

1. Buffer behaviour:
    a. More thorough review of Senna et al. (TR-10-59) than was possible during this initial review would establish more clearly the implications for coupled modelling of buffer resaturation and corrosion.

    b. More thorough review of Grandia et al. reports. (TR-10-25 and TR-10-62) than was possible during this initial review would establish more clearly the implications for coupled modelling of buffer resaturation and corrosion.

    c. The bentonite erosion mass transport model used in the corrosion calculations described in the **corrosion report** (TR-10-66) should be checked by reviewing the report **on mechanisms and models of bentonite erosion** (TR 09 35) and the report **on modelling of erosion of bentonite gel by gel/sol flow** (TR 10 64).

    d. The conceptualisation of fracture flow paths and their intersections with deposition holes, which underpins models of buffer resaturation in the **main report of the SR-Site project** (TR-11-01), needs to be reviewed in detail. The aim of the review would be to establish how alternative conceptualisations might influence the modelled resaturation of the buffer and consequently its performance. For example, if a fracture that intersects a deposition hole is modelled as a planar feature with uniform hydrogeological properties, resaturation will be predicted to occur differently to a case in which the fracture is modelled to as having heterogeneous hydrogeological properties (e.g. flow occurring along effectively 1D channels within the fracture plane).

2. Corrosion:
    a. The **corrosion report** (TR-10-66) and literature that supports it should be reviewed more thoroughly than was possible during the initial review reported in this document. The detailed review should focus on uncertainties in mathematical treatment of corrosion/erosion that were identified in this initial review. An assessment should be made of the implications of these uncertainties for the calculated probabilities of canisters experiencing corrosion over the full depth of the copper casing during the 1,000,000 y assessment period.

    b. The new Q_{eq} terms calculated by SKB to account for spalling should be checked by reviewing the report on **mass transfer between waste canister and water seeping in rock fractures** (TR-10-42).

3. Data from the DFN model is used in almost all EBS modelling activities, from buffer resaturation to corrosion. The way in which data from the DFN model has been used or post-processed to determine or inform choices of parameters is not always clear. Furthermore it is not apparent that conservatisms and uncertainties that have been investigated from a 'groundwater flow perspective' in the DFN modelling are appropriate conservatisms and uncertainties from the perspective of the various EBS modelling activities. The way in which uncertainties in the various modelling activities are related should be analysed and SKB's DFN reports should be reviewed in this context.

Areas requiring further analysis/modelling:

1. Resaturation / Homogenisation:

    a. Further THM modelling should be undertaken to improve the representation of the competing suction and permeability relationships as saturation varies within the bentonite. These new models should be carried out in 2D and should focus on more adequately accounting for observed full-scale resaturation in the CRT.

    b. After demonstrating that the CRT inflows can be adequately represented (item above), additional modelling should be undertaken to determine the change in the response to resaturation in the buffer when more realistic in-situ boundary conditions are applied. The modelling should investigate the plausibility and implications for buffer performance of long-lived heterogeneous buffer resaturation patterns. This modelling should be carried out in 2D and ideally would take into account chemical processes that will affect the buffer.

    c. Resaturation and swelling / homogenisation in buffers constructed with alternatives bentonite (Ibeco / FEBEX etc.) with varying monovalent:divalent cation ratios (compared to 3:1 for MX-80), should be investigated to determine how conclusions presented for MX-80 may differ for alternative bentonite.

    d. Potential hydrogeological interactions between neighbouring deposition holes should be investigated. For example, in a slow flowing fracture, the possibility for an 'upstream' deposition hole to draw water towards itself and deprive downstream deposition holes of water should be investigated. This could have the effect of reducing hydraulic heads below hydrostatic for long periods at fracture intersections with downstream holes.

2. Independent calculations to investigate corrosion / erosion:

   a. Additional calculations should be undertaken to confirm that the lowest groundwater salinities that could plausibly be attained (apparently equivalent to around twice the safety function indicator of total ionic strength of cations >4 mM) will not result in a significantly enhanced likelihood of buffer erosion.

   b. Validate the distribution of corrosion rates calculated by SKB, in particular to check that the Q_{eq} transport terms are sufficiently accurate or that the resulting transport rates are conservative;

   c. Check that simplifications and assumptions made in the derivation of Q_{eq} terms do not lead to inaccuracies when different geometrical configurations are assumed; and

   d. Check the use of the Buffer Concentration Factor (BCF), to confirm whether or not it underestimates the likely amounts of corrosion when fractures are located away from the canister mid-height (as is suggested by independent calculations) and / or are combined with spalling and unfavourable flow conditions.

3. Long-term chemical alteration of the buffer and backfill:

   a. Independent modelling to check Senna et al.(TR-10-59) should be undertaken to explore the significance of uncertainties connected with the redistribution of trace and minor mineralogical components within the buffer.

   b. Additional models should be undertaken to verify previous models of cement-bentonite interactions presented in reports on **evaluation of low-pH cement degradation** (TR-10-62) and **quantitative modelling of cement degradation processes (**TR-10-25). This verification should focus particularly on the sensitivity of these models to the kinetic rates that are assumed and the grid sizes employed. This additional work should include a thorough review of the thermodynamic data that have been used in these models.

4. **Modelling colloid generation and release:** Colloid generation in the buffer and subsequent release to the groundwater system were not considered in the present review. Additional modelling should be undertaken to verify SKB’s modelling of these processes taking into account possible heterogeneous buffer resaturation and plausible variations in groundwater chemistry.

Areas in which extra competence is needed in order to undertake review.

1. Additional competence is needed in the field of microbiology in order to review thoroughly the potential significance of biogeochemical processes that may operate in the buffer and backfill and their implications (if any) for canister corrosion.

APPENDIX 4

Detailed Comments on Reviewed Reports

TR-11-01: Main report of the SR-Site project

1. Page 65, 3rd bullet point states that resaturation of the buffer, the backfill and the host rock typically requires tens to hundreds of years “for Swedish conditions”. What does “Swedish conditions” mean in this context? The SR-Site report concerns Forsmark and therefore should give an indication of resaturation times at Forsmark. It would also be beneficial to indicate how these times are likely to vary across the site.

2. Page 134, para 3, line 2. It is stated that “Most of the Eh values determined in brackish groundwaters (at depth between 110 and 646 m) seem to be controlled by the occurrence of an amorphous iron oxyhydroxide with higher solubility than a truly crystalline phase. *This indicates that the iron system is disturbed*”. Why does this observation indicate a disturbed iron system? Is the intended meaning that the iron system is not at true thermodynamic equilibrium because amorphous iron oxyhydroxide is a metastable phase? The reference to “Most of the Eh values” being reducing needs clarification. This statement implies that some Eh values were not reducing. Hence it should be stated why these “oxidizing” Eh values have been rejected and the interpretation made that the water from this depth range is reducing.

3. Page 149, last sentence. It is stated that “When quantitative [function indicator] criteria are not given, the term “limited” is used to indicate favourable values of the safety function indicators. The term “limited” requires explanation since on its own it has no real meanning. For example, it is stated that salinity in terms of total dissolved solids (TDS) should be “limited”. Presumably this means that the TDS is insufficiently high to call into question the proper functioning of the buffer. It ought to be possible at least to give some indication as to the likely maximum TDS that would be acceptable.

4. Page 152, last paragraph. It is stated that “..for practical reasons, the old definition [of the Extended Full Perimeter Intersection Criterion], i.e. rejecting deposition holes intersected by a fracture also intersecting the full tunnel perimeter has not been altered for the far less frequent potentially water bearing fractures.”. Does this statement really refer to “water-bearing” fractures? Any fracture with open porosity would contain water and hence could be described as “water-bearing”, irrespective of the flux of water through the fracture. If the statement means instead to refer to flowing fractures it would be more appropriate to use “transmissive” rather than “water bearing”. It would also be helpful to state what is meant by “water bearing” (or alternatively “transmissive”) in this context. Presumably there is a groundwater flux criterion that would be applied (e.g. such that the total amount of water flowing into the accepted deposition hole would be <150 m^3, as stated on page 152, para 2 of TR-11-01)?

5. Page 158, para 5, line 1 states that “The successful application of the EFPC is also assumed for the hydrogeological simulations”. How is it known that the EFPC application has been “successful”?

6. Page 158, para 5 is rather confusing. It appears to be saying that some fractures that could result in the inflow criterion (0.1 L/min) being exceeded might not be identified, but “very large fractures” that would result in an inflow of 25L/min would be identified. This leaves the reader wondering how in fact unfavourable deposition positions would be recognized.

7. Page 251, last bullet point states that “A safety function indicator criterion is a quantitative limit…” However, not all safety function indicators are actually defined quantitatively. For example, Figure S-7 states that Safety Function R1. “Provide chemically favourable conditions” has the safety function criterion “Salinity; TDS limited”.

8. Page 254, para 17 states that “The buffer homogeneity is ensured partially by the fact that the buffer is made of a clay material that swells when water saturated”. There are many examples of heterogeneous clay materials and the fact that the buffer is made of clay is not, on its own, evidence that the buffer will be homogeneous.

9. Page 257, 5th bullet and sub-bullets states that “The following processes [Radiation attenuation/heat generation, Radiolysis of porewater”, Radiation-induced transformations, Liquefaction] have not led to the definition of safety functions since they were deemed as insignificant for long-term safety in the evaluation in the Buffer, backfill and closure process report”. It would be helpful to explain the reasons why these processes were deemed insignificant, in addition to referencing the buffer, backfill and closure process report.

10. Page 259, para 2, line 1 states that “In general, ionic strengths corresponding to NaCl concentrations of approximately 35 g/L (0.6 M NaCl) are an upper limit for maintaining backfill properties whereas the corresponding limit for the buffer is around 100 g/L (1.7 M NaCl)”. These limits are different to values that have been quoted elsewhere. For example, a report on **hydrochemical evolution of the Forsmark site** (TR-10-58) references SKB (2006) and states that “In general, ionic strengths corresponding to NaCl concentrations of approximately 1.2 M are a safe limit for maintaining backfill properties, whereas the corresponding limit for the buffer is around 1.7 M”.

11. Page 367, Section 10.3.8, line 4 states that “The water saturation process itself has therefore no direct impact on the safety functions of the buffer and backfill.” The argument made to support this statement is that under un-saturated conditions, no mass-transfer can occur between the canister and the groundwater in the rock. However, it is possible to envisage a case where the buffer surrounding a canister is not fully saturated, but portions of the buffer between the host rock and the canister are fully saturated. Additionally, if piping and erosion take place during the course of resaturation it could be argued that the resaturation process *does* have a direct impact on safety functions.

TR-10-11: THM modelling of buffer, backfill and other system components (2 volumes)

1. Page 15, Section 2.5. First para. refers to Section 2.4. Should be Section 2.3.
2. Page 19, Table 2-1. Grout degradation work in TR-10-25 used RCB (RETRASO + CODE_BRIGHT). The table only mentions CODE_BRIGHT.
3. Page 20, Table 2-2. Entry for TR-10-59 (Sena et al.) gives data as 1020. Should be 2010.
4. Page 371, Bullet 4 – states that a rock permeability of 1e-20 corresponds to a hydraulic conductivity of 1e-14. Using standard values for fluid density and viscosity, a difference in 7 orders of magnitude would be expected between these numbers.

TR-10-66: Corrosion calculations report for the safety assessment SR-Site

1. It is not clear whether the flow rate in a spalling zone, q_{zone}, which is given in Equation 4-8 on page 18, is actually calculated in the DFN models (are spalling zones represented in the DFN?) or whether are they inferred. Flows in spalling zones should be assessed as part of the DFN review.

2. Page 29, Section 5.2.3, para 3, line 6 mentions oxygen penetration to the “most exposed deposition position in the repository”. What is the meaning of “most exposed” in this context? Does it refer to the location where groundwater has the highest oxygen concentration, or where the groundwater flux is greatest? Alternatively, do these positions coincide?

3. The Q_{eq} diffusive term given in Equation 4-13 for the diffusive transport between the spalling zone and buffer assumes a Cartesian geometry. For a large spalling zone this is likely to be a reasonable approximation, but for a smaller or less well connected spalling zone a version derived in a cylindrical geometry may be more accurate.

4. Equation 4-15 appears to be wrong (it is a duplication of Equation 4 14). The caption given in TR-10-66 Figure 4-1 would seem to be the correct equation that was intended.

TR-10-59: Aspects of geochemical evolution of the SKB near field in the frame of SR-Site

1. General comment: The English is awkward in many places within the report and there are many typographical errors.

2. Page 7, para 9, line 3 and Page 8, Figure 1-1 describe the model cases used to investigate buffer and backfill evolution. The text states that Case 1 used a 3D model and Case 2 used a 2D model. However, the figure shows a 3D domain for Case 1 and a 2D plane for Case 1.

3. Page 12, Table 1-3 does not indicate the units. Presumably these are molal.

4. Page 23, para 1, line 3 states that “Like PHREEQC, PHAST is able to simulate multicomponent, reactive solute transport in three-dimensional saturated groundwater flow systems”. However, PHREEQC cannot simulate systems in 3-D.

TR-10-51: Model summary report for the safety assessment SR-Site

1. Section 3.2.6 is named “Rationales for using the code in SR-Can”. SR-Can here should be SR-Site.

TR-10-52 Data report for the safety assessment SR-Site

1. Section 5.3: How is potentially diffusion-dominated transport in the backfill handled?
2. Section 5.3.2, correlations used in SR-Can modelling: What is meant by saying that the correlations in SR-Can generally agree with those in SR-Site? Is this just saying that the same approach was used or that the same conclusion was reached?
3. Section 5.3.2, p 154: The final sentence is unclear. Does it just mean that some species were not in SR-Can?
4. Section 5.3.2, 3rd para: The question of which groundwater to use is discussed. Is the text on page 180 (under Conditions...) intended to address the question raised there? Has it been shown that using SR Site groundwater would not change the conclusions?
5. Section 5.3.5, 5th para. Why is the dry density of backfill in SR Can relevant?
6. Table 5.3 of this section gives the cation exchange capacity (CEC) of MX-80 bentonite as being 85 meq/100 g in the SR-Can assessement, but 75 meq / 100 g in the SR-Site assessment. The preceding paragraph implies that the difference is due to the different densities specified for the bentonite in the two assessments. The reason should be stated explicitly.
7. Sub-section on groundwater, page 158, 2nd para states that reference groundwaters in Ochs and Talerico (2004) included two alkaline variants, one with pH of up to 13.5. However, without the reader obtaining the original source, it is unclear how or why these variants were specified. A pH of 13.5 is very alkaline indeed. Presumably it is a cement porewater? An explanation is needed.
8. Section 5.3.5, last sentence of page 158. On what basis is the claim for 99.9% confidence limits made – is there enough data to support such a claim? In any case, why quote a confidence limit of 99.9%; why not quote 90%, 95% or 100%?
9. What is the rationale for recommending very wide ranges of Kd values for many elements, rather than recommending conservative values? The quoted ranges of Kd in TR-10-52 are often larger than ranges that have been recommended for use in safety assessments in other programmes and would give rise to non-conservative results when applied in transport calculations.
10. Page 159, 4th para states that “As the Finnsjön site is located nearby the Forsmark site, and in a broader sense has about the same geological settings, it is suggested to be acceptable to use the Kd data of Ochs and

Talerico (2004)”. It is reasonable to use the Finnsjön data for the stated reasons, but the reader will wonder why data are not available for Forsmark itself. Some clarification would be helpful. Additionally, the statement that “it is suggested to be acceptable” to use the Kd data is an example of many cases in this report where unclear recommendations are given. Why not state clearly that it is recommended to use these Kd values? The fact that it is only a suggestion will imply to many readers that there is uncertainty about whether in fact they should be used.

11. Page 160, 1st para of the section concerning pore water states that models need to be used to estimate pore water compositions because there are experimental and conceptual uncertainties in obtaining data directly from compacted bentonite. It is true that there are challenges associated with extracting porewater for analysis. However, it is still valuable to compare analyses of extracted porewater with model results. Was this done?
12. Page 161, 3rd bullet states that salinity does not have a marked effect on Kd for most species. While this is true for the range of salinities of relevance to SR-Site this salinity range should be stated explicitly.
13. Page 161, 9th para (counting bullets at paragraphs) states that “Interpolation between the three reference pore water conditions is easily possible for salinity, but should to be done with care for parameters that are directly linked to others (pH, pCO_2)”. The use of the term “with care” is another example of imprecise terminology. What does this mean? For parameters that vary non-linearly with mixing, such as pH and pCO_2, linear interpolation should not be used.
14. Page 161, para 13 (counting bullets at paragraphs) states that differences in pore water compositions, and hence Kd, between MX-80, Deponit CA-N, and Milos backfill are considered to be negligible “based on the available information”. What is this “available information”. A reference should be given.
15. Page 162, sub-section of Section 5.3.5 concerning the temperature-dependency of De states that an increase in temperature to 50°C is expected to lead to a twofold increase of De, while a decrease in temperature to just above freezing is expected to lead to a twofold decrease. What is the basis for this statement? A cross reference to Section 6.8.5 is provided, but this section also does not justify the quoted temperature dependence. At least some published literature seems to suggest a smaller variation, around a factor of 1.5 (e.g. Bastuk and Kuyucak, 2005).
16. Page 162, 2nd bullet of Section 5.3.6 states that “For Kd, the most significant conceptual uncertainties, *in terms of representing reality*, are related to the description of pore water composition as a function of conditions”. This statement is untrue. The most significant *conceptual* uncertainty concerns the validity of Kd itself. Limitations of the Kd concept are discussed in a number of sources to which reference should be made (e.g. McKinley and Alexander, 1993). The use of Kd assumes that there are an infinite number of sites on a sorbing surface at which a particular specie may sorb. In reality there will be a finite number of such sites. The Kd concept is therefore valid only if the sorbent has not been “saturated” with the sorbing species. Sorption isotherms, such as Langmuir isotherms are conceptually closer to reality. There should be a discussion of the advantages and limitations of the Kd concept within TR-10-52, but none is given.
17. Page 162, 2nd bullet of Section 5.3.6 also states that the composition of pore water composition in compacted bentonite cannot be determined experimentally with any certainty requires qualification. While there are

certainly challenges associated with obtaining pore water chemical data, it is feasible to obtain useful information that can be used as a guide to / check on models.

18. Page 163, para 5 of sub-section entitled “Neutral diffusants (HTO)” states that “Recommended De values are based on a regression analysis including all HTO data for Kunigel-V1 and MX-80”. Why were the Kunipia-F bentonite data not used? Presumably this was to ensure conservatism, noting that Kunipia-F is almost pure bentonite and hence gives lower De than the other, more impure bentonites?
19. Page 167, paragraph following Equation 5.4 states that “The resulting best estimate De values are 1.4 x 10^{-10} m^2/s for the buffer (ρd = 1,562 kg/m^3) and 1.6 x 10^{-10} m^2/s for the backfill (ρd = 1,504 kg/m^3)”. Given that the difference between these values is small compared to the large scatter in the De data shown in Figure 5-6, it is unjustified to recommend different values for the backfill and the buffer.
20. Page 167, 1st bullet point in the sub-section entitled “Anions” states that “Accepting the argumentation in Ochs and Talerico (2004), it is suggested that the model prediction by Ochs et al. (2001) for the diffusion of chloride in MX-80 is representative for the range of dry densities considered here”. Given that the arguments in Ochs and Talerico (2004) are important, they should be summarized here.
21. Page 167, 1st bullet point gives best estimate De values of 1.1 x 10^{-11} m^2/s for and 1.2 x 10^{-11} m^2/s for the buffer and backfill respectively. Again, given the fact that the difference between these values is so small compared with the scatter in the data it is unjustified to recommend different De for the buffer and backfill.
22. Page 167, 2nd bullet states that “Upper and lower limits are somewhat subjectively based….”. This is another example of unclear English. The values are either chosen subjectively or objectively, they cannot be “somewhat subjective”. Some indication should be given of the potential significance for overall uncertainty of the subjective judgements that were made, otherwise this statement is unhelpful to any reader.
23. Page 167, para 5 (counting bullet points as paragraphs) states that “By taking this approach, the uncertainty ranges become rather large. ***It is therefore suggested*** that they also encompasses the minor deviations in dry density estimated for the buffer and backfill”. The use of the phrase “It is therefore suggested that” leaves the reader wondering what was actually done.
24. Page 168, Figure 5-9 gives green lines that bound most of the De data. The caption states that the green lines were placed subjectively. The criteria adopted for making these subjective judgements should be stated clearly. Several data points plot just outside the delineated fields causing the reader to wonder why the green lines were not drawn to enclose them too.
25. Page 168, 2nd para of the sub-section entitled “Caesium” states that “We refrain from speculating whether this spread [in De] is due to errors (experimental, raw data interpretation, etc.)”. The reader is caused to wonder why no speculation is made. It would be better to state simply that the reasons are unknown.
26. Page 168, 3rd para of the sub-section entitled “Caesium” gives De for caesium in the buffer and backfill of 4.2 x 10^{-10} m^2/s and 4.8 x 10^{-10} m^2/s respectively. Again, given the uncertainties in De measurements and the fact that these values are quite similar the validity of specifying different De for the buffer and backfill is questionable. Presumably the Kinipia-F

data are again ignored when deriving De in order to be conservative? It should be stated explicitly whether or not this was the case.

27. Page 168, 1st para sub-section entitled “Diffusion-available porosity” mentions “an explicit effort to distinguish De from ε”. However, De is effective diffusivity whereas ε is diffusion-accessible porosity. It would be better to state that an explicit effort was made to distinguish the *effects* of variable De from the *effects* of variable ε.
28. Page 168, 1st para sub-section entitled “Diffusion-available porosity” reports that published diffusion-available porosities for Cl are a factor of 1.8–3.5 smaller than for HTO. It is then proposed to use a reduction factor of 2.5 based on these data. The fact that the value of 2.5 is only “proposed” again causes the reader to wonder what value was in fact used. This report should clearly specify values for use in the assessment. Additionally, the arithmetic mean of 1.8 and 3.5 is 2.65. Hence, why was a value of 2.5 recommended? While perhaps a minor issue, this case illustrates the inconsistent approaches adopted in this report when recommending parameter values for use in the assessment. In earlier sections, as noted above, the report distinguishes between De values for buffer and backfill, even though the differences between the quoted values for the different materials are smaller than the uncertainties in the data. In contrast, here rounding appears to have been done which seems to cause a relatively large deviation between the actual mean of the data and the recommended value.
29. Page 170, 2nd para states that “Based on the available data, the compositions of Deponit CA-N and Milos bentonites are relatively similar to that of MX-80”. What is the meaning of “*relatively* similar”? Presumably this statement concerns the mineralogical compositions of the different bentonites (montmorillonite, quartz etc) since they have different exchangeable cation populations. The paragraph continues to state that “Therefore, it can be expected that calculated pore water compositions will be similar, in particular under conditions where carbonate equilibria are controlled by an external pCO_2 (open system)”. Given the different exchangeable cations in the different bentonites (dominantly Na in MX-80 and Ca in the others) it would be expected that the pore water compositions would differ to some degree in the different materials.
30. Page 170, 2nd para of the sub-section on uncertainty factors (UF) states that the UF-starting Kd is set to ±0.4 log10 units or ±0.6 log10 units, depending respectively upon whether an analogue element shows similar or dissimilar speciation to the element for which Kd is required. What is the justification for these values?
31. Page 171, 5th para states that the large uncertainty ranges in Kd should not give rise to non-conservatism in probabilistic modelling, “as it is the lower tail of the Kd distribution that affects assessment results”. This statement is unclear. If the upper estimates of Kd are higher than experimentally observed, presumably they give rise to greater nuclide retardation and hence reduced risk? How is it that the "lower tail of the Kd distribution" is more important?
32. Page 171, Figure 5-1, caption should state clearly that the coloured circles represent the modelled Da values and reiterate the explanations of RPW, RPWC and HSPW.
33. Page 172, 5th bullet point references Ochs and Talerico (2004) for details of the selection of UF for Cd and Ni. It is inconsistent with the detailed discussion of other UF in earlier sections simply to reference another literature source without giving details here.

34. Page 172, 6th bullet point concerns the Kd values for sulphur and gives a Kd value of 5 x 10^{-4} m^3/kg for SO_4. The validity of this Kd is questionable. Given that so few data exist and given evidence for weak sorption, it would be more reasonable to recommend conservatively that SO_4 should be treated as non-sorbing. Other programmes have not treated SO_4 as a sorbing. In any case, the buffer material contains trace gypsum, which means that probably SO_4 concentrations will be solubility limited, at least for a substantial period of the buffer's evolution. In this case, it will be invalid to use the Kd approach anyway.
35. Page 173, Figure 5-12 shows no units for the sum of dissolved chloride and sulphate which are labelled against the x-axis. Presumably molal units are plotted?
36. Page 173, 1st para of sub-section on temporal variability of data indicates the Kd data that should be used "If the post-closure removal is limited…". Presumably this statement refers to post-closure removal of buffer?
37. Page 173, 2nd para of sub-section on temporal variability of data unusually states that "one must be humble to the fact". This is not a normal turn of phase in an English language technical document.
38. Page 174, Section 5.3.9, point 9 states that the weakly sorbing ion CO_3^{2-} will not correlate. Even accepting that CO_3^{2-} will sorb, the Kd approach is invalid if the specie is solubility-limited, which must be likely given the occurrence of calcite. Once again, there should be some discussion of the validity of the Kd concept.
39. Page 176, 2nd para states that "The number of significant digits in the Kd values are taken directly from Ochs and Talerico (2004) and does not reflect the accuracy with which the data are estimated". It would be better to quote a number of significant figures that is commensurate with the precision of the data.
40. Page 176, Table 5-16 gives Kd values. These have been compared with values given for MX-80 bentonite in Bradbury, M and Baeyens B (2002). In the cases of most elements, the values in Bradbury and Baeyens lie within the ranges quoted in Table 5-16. However, in most cases the ranges in Table 5-16 are wider. The fact that very high upper limits (in comparison with the lower limits and with values in other compilations) are given for many elements in Table 5-16 raises a concern that risk dilution may be a problem in the assessment calculations that use these values.
41. Page 179, 1st para again states that SO_4 is assumed to be slightly sorbing. The validity of this assumption, and indeed its relevance in the context of the assessment, is questionable. It would be better to treat SO_4 as being non-sorbing.

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The Swedish Radiation Safety Authority has a comprehensive responsibility to ensure that society is safe from the effects of radiation. The Authority works to achieve radiation safety in a number of areas: nuclear power, medical care as well as commercial products and services. The Authority also works to achieve protection from natural radiation and to increase the level of radiation safety internationally.

The Swedish Radiation Safety Authority works proactively and preventively to protect people and the environment from the harmful effects of radiation, now and in the future. The Authority issues regulations and supervises compliance, while also supporting research, providing training and information, and issuing advice. Often, activities involving radiation require licences issued by the Authority. The Swedish Radiation Safety Authority maintains emergency preparedness around the clock with the aim of limiting the aftermath of radiation accidents and the unintentional spreading of radioactive substances. The Authority participates in international co-operation in order to promote radiation safety and finances projects aiming to raise the level of radiation safety in certain Eastern European countries.

The Authority reports to the Ministry of the Environment and has around 270 employees with competencies in the fields of engineering, natural and behavioural sciences, law, economics and communications. We have received quality, environmental and working environment certification.

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