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Overall evaluation of Tasks 8A–D, F, and water-uptake test related to modelling of the interaction between engineered and natural barriers

Task 8 of SKB Task Forces EBS and GWFTS

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Keywords: Äspö Hard Rock Laboratory, BRIE, SKB Task Force, Groundwater flow, Fractured rock, Bentonite, Interaction EBS-NS, Numerical modelling, Deposition hole.

Abstract

This evaluation report is a critical assessment of the work performed by the eleven modelling groups that participated in Task 8 of the SKB Task Force on Groundwater Flow and Transport of Solutes and Engineered Barrier Systems. Task 8 used numerical modelling and data from the Bentonite Rock Interaction Experiment (BRIE) to study water flow from the fractured rock into the bentonite buffer in a deposition hole, and to examine water redistribution within the bentonite, which impacts the timing needed for complete hydration. Different simulators, conceptual models, and coupling strategies were employed to capture saturated flow in the fracture network, partially saturated flow in the bentonite, and the interaction between these two subsystems. The analyses performed by the modelling groups yielded valuable insights, specifically regarding the relative importance of fractured-rock characterization and bentonite wetting behaviour. While the modelling groups arrived at different views about some aspects of the problem, both their agreements and differences led to an improved overall understanding of the interaction between the natural and engineered barrier systems. Moreover, it provided the basis for a comparative analysis that examined conceptual model uncertainty. Task 8 also demonstrated that a strong link between numerical modelling and laboratory or field experimentation is of great value. Both activities benefit from each other if part of the modelling is dedicated to supporting experimental design, and if testing and monitoring generate data that help to test hypotheses and discriminate among alternative conceptualisations.

Sammanfattning

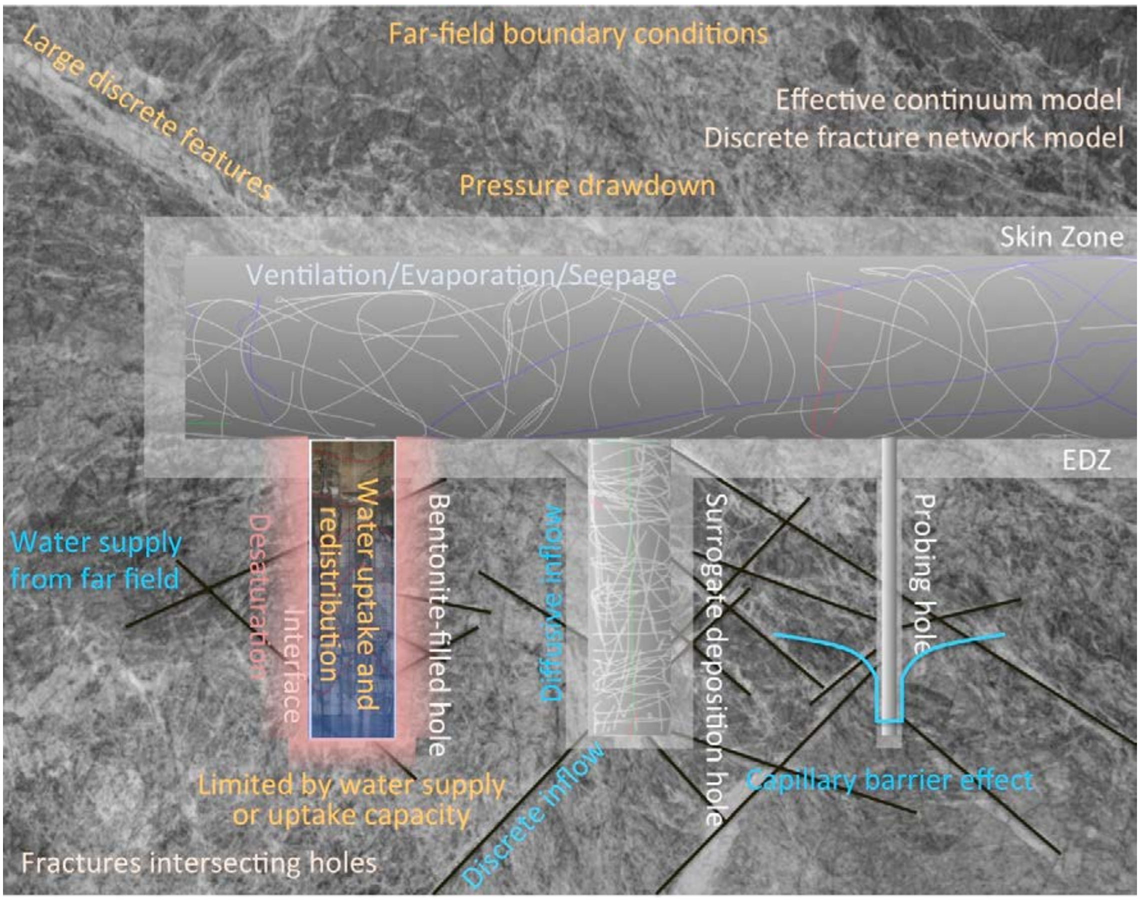
Denna utvärderingsrapport ger en kritisk bedömning av det arbete som utförts av de elva modelleringsgrupperna som deltog i modelleringsuppgiften Task 8 inom SKB: s internationella arbetsgrupper (Task Forces) för grundvattenflöde och transport av lösta ämnen samt ingenjörsbarriärsystem. Inom Task 8 används numerisk modellering och data från Bentonite Rock Interaction Experiment (BRIE) för att studera vattenflöde från det sprickiga berg som omger bentonitbufferten i ett deponeringshål samt för att undersöka vattenfördelningen i bentoniten, vilket inverkar på den tid som krävs för fullständig bevätning. Olika modelleringsverktyg, konceptuella modeller och kopplingsstrategier användes för att simulera mättat flöde i spricknätverket, delvis mättat flöde i bentoniten samt interaktionen mellan dessa två delsystem. Analyserna som utfördes av modelleringsgrupperna gav värdefulla insikter, speciellt angående den relativa betydelsen av karakterisering av sprickigt berg och bentonitvätningsbeteende. Emedan modelleringsgrupperna kom till olika åsikter om vissa aspekter av problemet ledde både dessa likheter och skillnader till en förbättrad övergripande förståelse för samspelet mellan de naturliga och konstruerade barriärsystemen. Dessutom gav detta grunden till en jämförande analys rörande konceptuell osäkerhet. Task 8 visade också att en stark länk mellan numerisk modellering och laboratorie- eller fältförsök har stor betydelse. Båda verksamheterna gagnar varandra speciellt om en del av modelleringen är avsedd att stödja experimentell design samt om testning och övervakning genererar data som hjälper till att testa hypoteser och diskriminera bland alternativa konceptualiseringar.

Executive summary

This evaluation report is a critical assessment of the work performed by the eleven modelling groups that participated in Task 8 of the SKB Task Force on Groundwater Flow and Transport of Solutes and Engineered Barrier Systems.

Task 8 was concerned with the hydraulic interaction between the natural and engineered barrier systems. The overall objective was to obtain a better understanding of the exchange of water across the interface between the fractured near-field bedrock and the bentonite buffer in a deposition hole for nuclear waste. Task 8 is related to the Bentonite Rock Interaction Experiment (BRIE; Fransson et al. 2017) at the Äspö Hard Rock Laboratory, which investigates inflow into open and backfilled surrogate deposition holes through field experimentation.

The schematic below shows the key elements of the natural and engineered system investigated by the Task 8 modelling groups, and summarizes some of the main issues that needed to be addressed. The can be described as follows:



The key modelling challenges included the development of a model that was capable of simulating flow of water through the fractured rock as well as hydration of the initially partially saturated bentonite. The interaction between these two subsystems was identified as the central element to be investigated, as effective bentonite wetting relies on sufficient water being supplied by the geologic formation. Moreover, the pattern of water supply at the interface has a significant impact on the uniformity and time needed for bentonite hydration.

The task description provided characterisation data from previous site investigations and modelling studies of the BRIE test bed. It also suggested parametric models to be used and prescribed performance measures to be evaluated. A series of subtasks was defined, each asking for predictions of inflow into open surrogate deposition holes and simulations of the bentonite hydration process, whereby the data made available from BRIE are to be assimilated into the modelling.

Based on the common set of characterisation data, the modelling groups developed alternative conceptual models that were implemented using a variety of numerical simulation tools. In particular, different approaches were developed to represent the fractured rock, which then needed to be integrated into or coupled with an appropriate model of the bentonite, where partially saturated or two-phase flow conditions prevailed. The resulting geosphere models ranged from classic discrete fracture network models, to heterogeneous effective continuum models, to hybrid models. The geosphere models were either fully integrated with a continuum model of the buffer, or run separately, or coupled using one-way or an iterative, two-way coupling strategy.

While no formal inversion approach was used, the modelling groups adjusted geometric and hydraulic parameters in attempts to improve the model fits to the measured BRIE data. In particular, stochastic fracture networks were conditioned to observed fracture traces, and special regions were introduced to reflect changed properties near underground openings. Multiple realisations of the stochastic fracture network were generated and simulated, and various sensitivity analyses were performed. Model development, simulation results, as well as related analyses and interpretations were presented at Task Force meetings and workshops, and documented in individual project reports (most of them are also published as separate SKB reports). These final reports were reviewed individually, and they formed the basis for a preliminary comparative analysis and overall evaluation of Task 8.

The analyses performed by the modelling groups yielded valuable insights, including the following:

- The behaviour of the combined geosphere-bentonite system can be categorized as either dominated by the limited water supply from the fractured rock, or by the limited water-uptake capacity of the bentonite.
- Bentonite wetting is driven by the bentonite properties and by the pattern of discrete inflow points, i.e. by local properties of the fractured rock.
- Measuring total inflows into a probing or deposition hole is of limited value for predicting bentonite hydration, because bentonite hydration may be controlled by bentonite properties rather than water supply rates from the formation.
- For the purpose of predicting bentonite hydration in a surrogate deposition hole under isothermal conditions, the bentonite can be treated as a conventional porous medium.
- Model calibration is challenging due to inherent non-uniqueness as well as uncertainties, simplifications, and errors in the conceptual model, and large variabilities and uncertainties in data and properties.
- Simulation tools are available to study the coupled behaviour of two subsystems with different key processes.

The modelling groups reached inconsistent or opposing conclusions on some aspects of the system, specifically regarding the significance or representation of the rock mass between discrete fractures (note that this rock mass consists of matrix, micro-fractures, and all fractures not explicitly represented in the model), and the need for accurate far-field characterisation.

The following overall evaluation comments were made:

- The work of the Task 8 modelling groups contributed to an improved understanding of the factors that affect the wetting of the bentonite buffer in deposition holes emplaced in fractured granitic rock. These insights were gained with support from data collected during BRIE and the related water-uptake tests. While the modelling groups arrived at different views about some aspects of the system, both their agreements and differences led to an improved overall understanding.
- The value of the modelling work could be further increased by examining the numerical results with focus on specific hypotheses that were (or need to be) formulated to better understand bentonite-rock interactions.
- The Task 8 work developed conceptual models, simulation tools, approaches and workflows that can be used to effectively target scientific questions of practical relevance for nuclear waste disposal in backfilled deposition holes. Now that the tools are available, future studies may focus more on the interpretation of the modelling results.
- The exchange of information and discussions during the Task Force meetings and workshops were dynamic, friendly, and professional, providing a solid basis for the overall success of Task 8.

The following recommendations were made:

- A conscious decision is to be made about how prescriptive the task description should be. This decision should be based on the technical objectives, but also accounting for the concept and goals of the Task Force as a whole.
- In the Task Force, multiple modelling groups address the same issues related to the interaction between the natural and engineered barrier systems. However, these issues were examined based on the group's specific areas of expertise and using different conceptual models, methods, tools, and interpretations. Moreover, the modelling groups (with one exception) provided results for only a subset of the tasks, which further reduced the overlap among the individual studies. For the Task Force to become more than a collection of individual modelling studies, it would be very valuable to encourage the groups to participate in a comparative analysis that provides a new perspective on broader lessons learned, unresolved issues, and conceptual uncertainties. It is recommended to make this comparative analysis an integral part of the Task Force by explicitly including it in the task description. For example, each group would dedicate a member to collaborate with the other modelling groups on the comparative analysis from the beginning of the project. This would have the following advantages:
    - Project objectives would be clearly articulated, and a list of testable hypotheses would be formulated.
    - The conceptual model and associated modelling assumptions would be clearly documented and communicated to the other modelling groups.
    - The risk that working towards a comparative analysis would lead to a more uniform set of alternative conceptual models could be mitigated by requiring that models deviate from each other by at least one key conceptual assumption. These differences could then be examined and used to discriminate among competing hypotheses, to the benefit of all modelling groups.
    - The need for informative performance measures would be apparent, and modelling results would be documented in a concise and complete manner.
    - The basis for a broader sensitivity analysis could be created.
    - Insights into the relative importance of data, parametric, and conceptual model uncertainties would be gained.
    - Modelling results would be interpreted and conclusions would be drawn with a more focused view on the common, overall objectives.
    - Participation in an overarching comparative study would encourage collaboration and information exchange among the modelling groups. It may also motivate timely reporting of modelling results.
    - Comparative analyses may lead to well-cited publications in the scientific literature.

- The Task Force projects are placed within the context of nuclear waste disposal. Uncertainty is an inherent aspect of this area of science and technology, regardless whether a specific Task Force project is concerned with research of fundamental processes, site characterisation, or performance assessment. Uncertainty (its description, quantification, and propagation) should thus be an integral part of the project from its beginning, with related guiding questions explicitly included in the task description.
- A strong link between numerical modelling and laboratory or field experimentation is of great value. Both activities benefit from each other if one part of the modelling is dedicated to supporting experimental design, and if testing and monitoring generate data that help a) calibrate the models, b) discriminate among alternative conceptualisations, and c) test hypotheses. A successful interaction between numerical modelling and physical experimentation requires considerable planning and coordination, and the willingness to adjust one's work scope to support the other team. Such cooperation may be facilitated by the Task Force Secretariat and outlined in the task description.
- If considered helpful and with the consent of the modelling groups, an annotated outline of the final modelling report could be provided early on. One might consider making this outline follow the general structure of a research paper (rather than that of a project report) to facilitate and encourage publication of the Task Force work in the scientific literature.
- A lecture or seminar by an outside expert on a topic of relevance to the Task Force work could be useful and stimulating. This expert may also be willing to participate in parts of a Task Force meeting and provide feedback.

This report has been reviewed by the modelling groups and the SKB Task Force management. However, the opinions and specifically the evaluation comments are those of the author.

Contents

1 Introduction

1.1 Background

The SKB Modelling Task Force is a forum for international organizations to interact in the area of conceptual and numerical modelling of groundwater flow and solute transport in fractured rock as well as of engineered barrier systems.

Task 8 is a joint effort of the SKB Task Force on Modelling Groundwater Flow and Transport of Solutes (GWFTS) and that on Engineered Barrier Systems (EBS). The overall objective of Task 8 is to obtain a better understanding (through modelling and analyses) of the hydraulic interaction between the near-field bedrock and backfill materials in the repository, specifically the bentonite buffer in a deposition hole.

Conceptual and numerical model development is based on insights gained from previous Task Force modelling studies, as well as on various experimental and analytical work performed at the Äspö Hard Rock Laboratory. Specifically, Task 8 is related to the Bentonite Rock Interaction Experiment (BRIE), which addresses the hydraulic interaction between the system components of compacted bentonite and the near-field fractured bedrock. The BRIE experiment is located in the short TASO tunnel, where vertical test boreholes were drilled for initial characterization and screening. The test boreholes were then widened (becoming surrogate deposition holes) to accommodate pre-compacted and instrumented bentonite blocks. (Note that in this report the term "deposition hole" refers to the 0.3 m diameter, open or bentonite-filled surrogate deposition holes at the BRIE site; see Appendix C for a glossary of terms used in this report.) The BRIE field experiment is complemented by a radial water-uptake laboratory test (Vidstrand et al. 2017). The experimental work complementing the modelling exercises of Task 8 are summarized in Section 1.3; details can be found in Fransson et al. (2017).

Task 8 modelling work and the BRIE experiments are interlinked in that the modelling can be used to support the design of the laboratory and field experiments, whereas the experiments provide characterization data, a basis for modelling scenarios as well as data that can be used to evaluate the conceptual appropriateness, explanatory capability, and predictive power of the numerical models.

The interaction between the bedrock and the engineered barrier system involves complex two-way processes. Their understanding and predictability critically depends on the underlying conceptual model, the available characterization data, the features and processes considered, and the details of their implementation in a numerical model. Moreover, it is essential to assess the impact of each model element on the results of interest, and how they in turn affect the conclusions and recommendations derived from these numerical studies. To examine the robustness and uncertainties of the models, different concepts and modelling approaches were developed by several modelling groups that ideally address the same questions related to a well-defined overall objective. The combined results of all modelling studies are likely to increase understanding of the features and processes governing bentonite-rock interaction, and a cross-comparison of the groups' findings may provide some insights into the variability and uncertainty inherent in such analyses.

Task 8 was structured into subtasks. Following a scoping calculation (Task 8A), the BRIE experiment was modelled in four stages with increasing complexity, incorporating more experimental data as they became available. These four stages are referred to as Tasks 8B–8D and 8F; they are described in more detail in Section 1.5 (Task 8E is concerned with the simulation of interaction effects on the scale of the Prototype Repository; Task 8E is not part of this evaluation report). All subtasks involve the modelling of both flow in the fractured bedrock and inflow into surrogate deposition holes that are either open or backfilled with bentonite. In addition, the laboratory water-uptake test (WUT) performed by Clay Technology AB (Vidstrand et al. 2017) provided additional characterization data and insights into the wetting behaviour of the bentonite; separate numerical models were developed to analyse the data and to increase confidence in the representation of the bentonite in the models developed of BRIE for Tasks 8B–8D and 8F.

This report summarizes the work performed by the modelling groups on Subtasks 8A through 8D, 8F, and the water-uptake test, and provides some comments on the analysis approach and results, as well as recommendations regarding future Task Force projects and analyses of rock-bentonite interactions. It also attempts to integrate and compare the results to the extent possible to assess the range of outcomes.

1.2 Rock-bentonite interactions

Figure 1-1 shows the key elements of the natural and engineered system investigated by the Task 8 modelling groups, and summarizes some of the main issues that needed to be addressed. They can be described as follows:

- The model represents a finite region of fractured granitic rock that contains multiple engineered underground structures.
- The granite contains fractures and other discrete geologic structures on multiple scales. They may be represented using:
  - A continuum model with effective properties.
  - A stochastic discrete fracture network (DFN) model.
  - A continuum model with large, discrete geologic structures implemented deterministically.
  - A DFN model with large, discrete geologic structures implemented deterministically.
  - A hybrid model, combining continuum and discrete models, with fractures implemented deterministically or using stochastic methods; specifically, fractures intersecting underground openings may be represented as deterministic, discrete geologic structures.
- Boundary conditions need to be specified at the outer model domain boundaries and the walls of underground openings.
- The TASO tunnel must be represented. A near-field pressure drawdown has developed due to long-term water seepage into the tunnel.
- Small-diameter probing holes (used for initial characterisation) need to be represented; they may be open or closed for hydraulic testing.
- Surrogate deposition holes need to be represented; these larger-diameter (300 mm) holes are initially open but eventually filled with bentonite.
- Skin zones around all underground openings may have developed because of mechanical effects, dry-out due to evaporation, desaturation due to suction by the bentonite, or other mechanisms. Specifically, an excavation damage zone (EDZ) with increased fracture apertures develops at the floor of the large tunnel, mostly attributed to higher explosive energy applied in blast holes close to the tunnel floor.
- Inflow into open holes needs to be simulated, accounting for a potential seepage face due to the capillary pressure effect.
- Inflow into open or bentonite-filled holes occurs through discrete geologic structures and through the rock mass between these features.
- Hydraulic properties and connectivity of the fracture network determines the amount of water being supplied to the fractures intersecting the open or bentonite-filled holes.
- Interactions between the fractured rock and the bentonite occur through an interface between the surrogate deposition hole wall and the bentonite. Feedback mechanisms between the two systems across this interface may be relevant.
- Capillary and pressure forces drive water entering the bentonite; water imbibition is potentially affected by local desaturation and other skin effects.
- Water that entered the hole non-uniformly through the interface is redistributed within the bentonite.

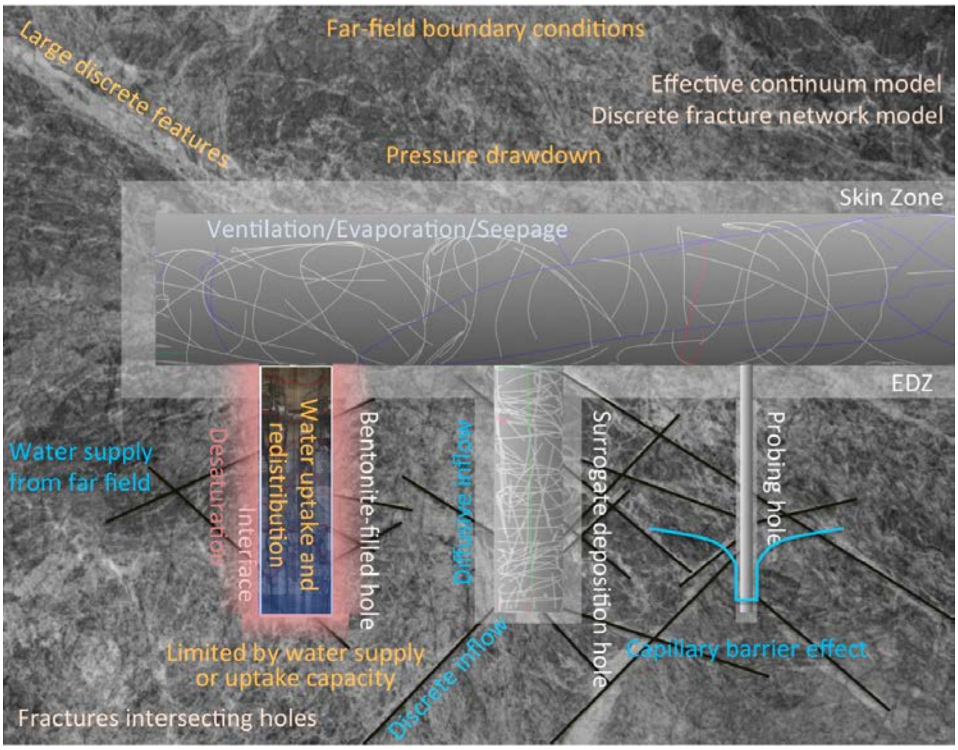


Figure 1-1. *Schematic of key system elements, processes, and modelling issues.*

1.3 The Bentonite Rock Interaction Experiment (BRIE) and water-uptake test

With the specific goal to examine how the characteristics of the fractured bedrock affect the wetting of the compacted bentonite used as buffer material in a deposition hole, Task 8 targeted a configuration representing the Bentonite Rock Interaction Experiment (BRIE), which started in 2010 at the Äspö Hard Rock Laboratory, located near Oskarshamn in south-eastern Sweden. BRIE addresses the hydraulic interaction between compacted bentonite and the near-field fractured bedrock. The main objectives of BRIE were to obtain:

- An increased scientific understanding of the exchange of water across the bentonite-rock interface.
- Better predictions of the wetting of the bentonite buffer.
- Better characterisation methods for the deposition holes.

These experimental objectives overlap with the objectives of the Task 8 modelling studies (see Section 1.5.1).

The BRIE experiment is located in the short TASO tunnel at a depth of approximately 420 m. Site investigations included three characterisation phases, which resulted in an integrated geologic and hydrogeologic framework model that described key processes, geometry of man-made and (hydro) geological structures (including geostatistical properties of the stochastic fracture network), material properties from core samples and field testing, and boundary conditions. The TASO tunnel is hosted in rather massive, medium-grained diorite, with some gabbroic volumes in addition to volumetrically significant granitic dykes and smaller, irregularly shaped granitic intrusions. Vertical probing boreholes (76 mm diameter) were drilled for initial characterization and screening. Inflow to these probing holes was measured, and the two central boreholes – KO0017G01 (Hole 17) and KO0018G01 (Hole 18) – were then widened to a diameter of 300 mm to become surrogate deposition holes. They had a length of approximately 3.5 m and 3.0 m, respectively. Information concerning rock type, fracture orientation, fracture filling, was obtained through core mapping supported by Borehole Image Processing System (BIPS; Gustafsson 2013) measurements (see Figure 1-3). Distribution and total inflows to the open holes were also measured by means of so-called “nappy tests”. A sketch of the key features at the BRIE site is shown in Figure 1-4.

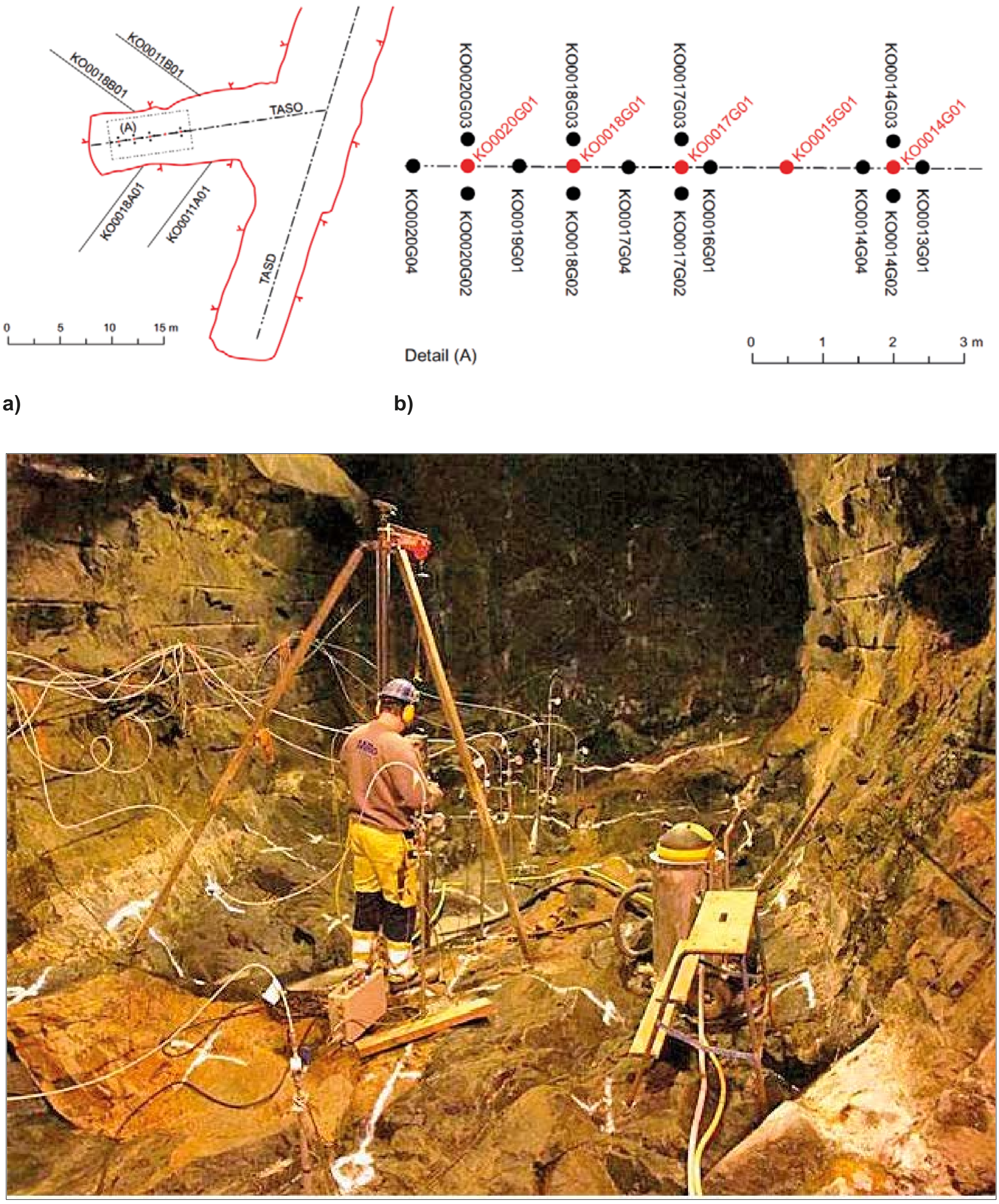


Figure 1-2. *a) Boreholes in tunnel wall and location of BRIE test bed; b) probing holes; boreholes KO0017G01 and KO0018G01 had their diameters increased from 76 to 300 mm, becoming "surrogate deposition holes"; c) BRIE test bed in TASO tunnel (Fransson et al. 2017).*

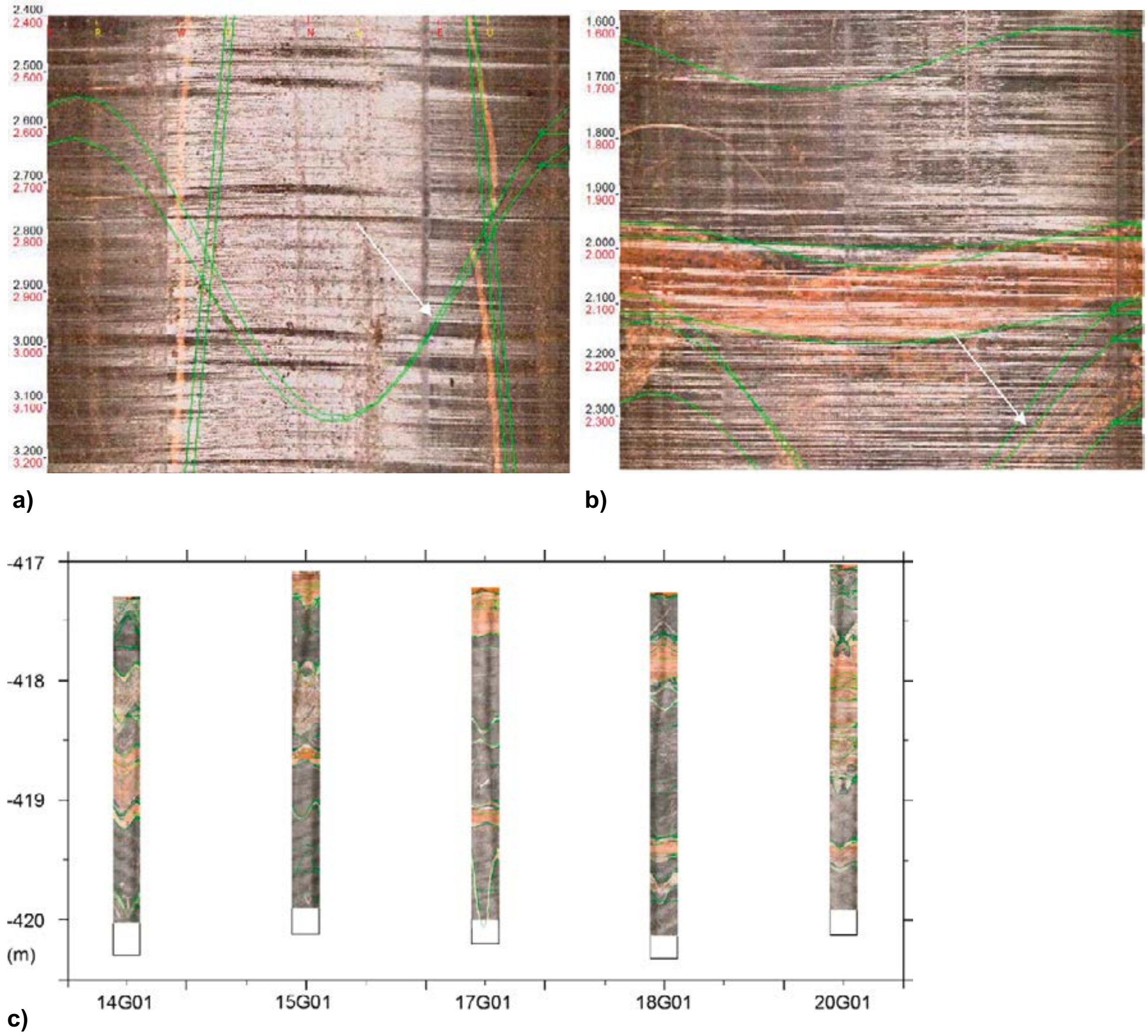


Figure 1-3. Borehole Image Processing System (BIPS) images for borehole a) KO0017G01 and b) KO0018G01; c) compilation of BIPS-images (Fransson et al. 2017).

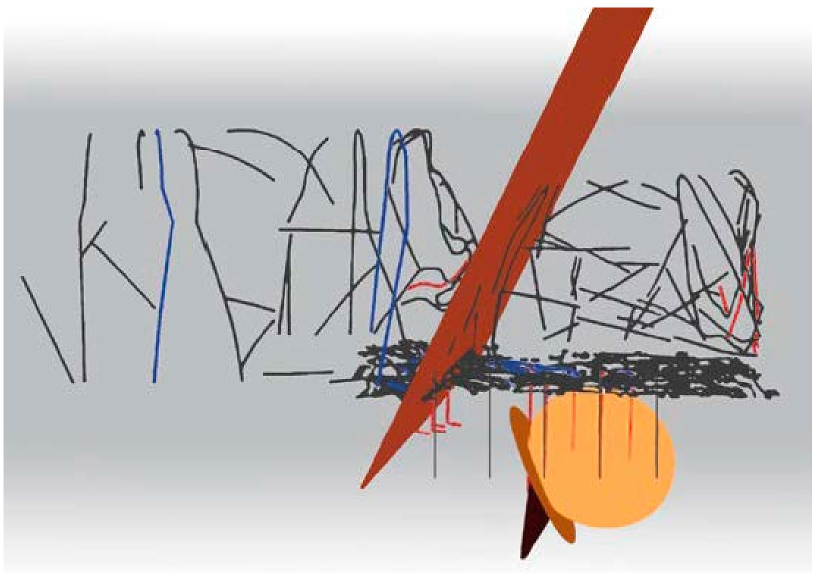


Figure 1-4. Sketch of the BRIE site including main water-bearing fractures and matrix in the central boreholes KO0017G01 and KO0018G01, the deformation zone identified in the middle of the tunnel and an excavation damaged zone (EDZ) (Fransson et al. 2017).

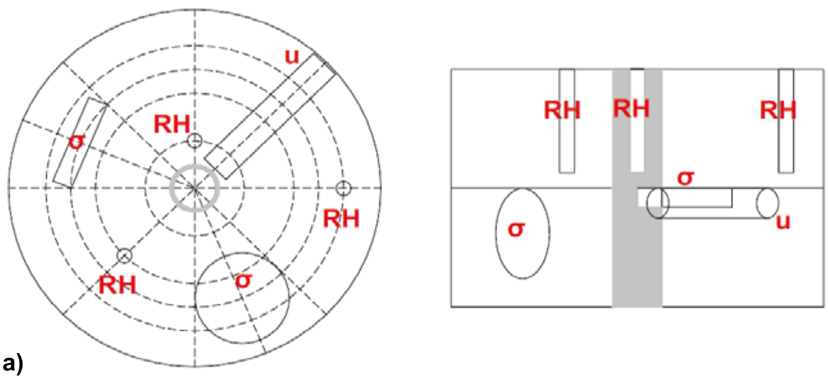
In September 2012, pre-compacted and instrumented bentonite blocks (see Figure 1-5) were installed in the surrogate deposition holes (see Figure 1-6). The bentonite parcels were instrumented with sensors that monitored relative humidity, axial- and radial total pressure as well as pore pressure. During installation, the central tube was accidently flushed, whereas the gap between the bentonite and the rock were intentionally filled with water.

Investigations for each of the central holes focussed on one section expected to be wet (close to a water-bearing fracture), and one section expected to be (comparatively) dry (not being close to a fracture).

Holes 17 and 18 were dismantled by stitch drilling and wire-line sawing in November 2013 and February 2014, respectively. The bentonite and the rock in contact with the bentonite (i.e. the wall of the central boreholes) were characterised and sampled to obtain water content, density and relative humidity data. Additional laboratory tests were performed providing hydraulic conductivity and water retention curves for the rock matrix. In addition, the retrieved bentonite was photographed to document traces of water-bearing fractures. One of these so-called "bentographs" is shown in Figure 1-7, along with interpolated water-content data.

BRIE led to valuable investigations and characterisation methods for rock and bentonite alike, and provided a unique data set for a heterogeneous, i.e. low-permeability rock matrix intersected by low-transmissive fractures as well as larger water-bearing features. A desaturated zone around the borehole was identified.

The BRIE site, experimental procedures and results are fully documented in Fransson et al. (2017).



a)

b) c)

Figure 1-5. a) Outline of sensor positions in instrumented blocks. RH: relative humidity, σ: total pressure and u: pore pressure; instrumentation of blocks: b) block with pressures sensors, and c) block with RH sensors (Fransson et al. 2017).

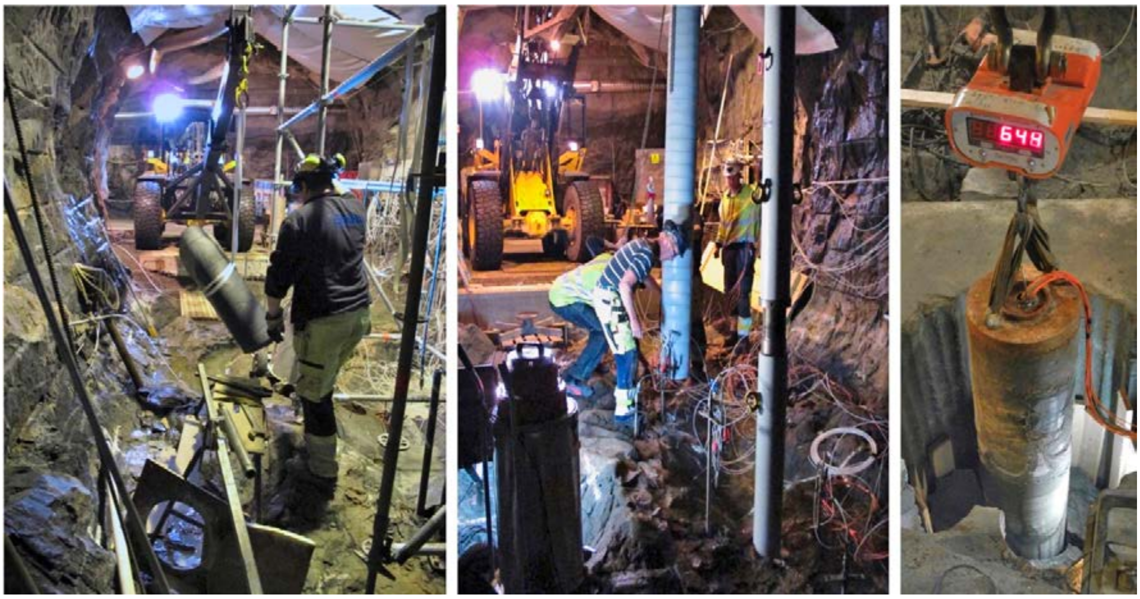


Figure 1-6. *The BRIE site in the TASO tunnel: drilling of the 300 mm boreholes (left), emplacement of the 3 m bentonite blocks (middle), extraction of bentonite blocks after 17 months (right) (Fransson et al. 2017).*

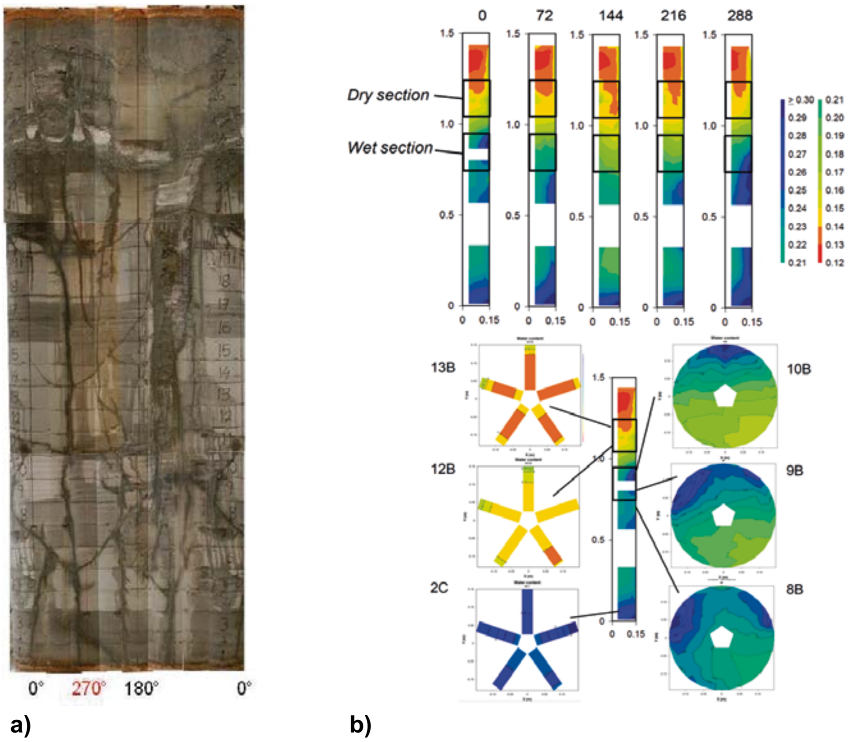
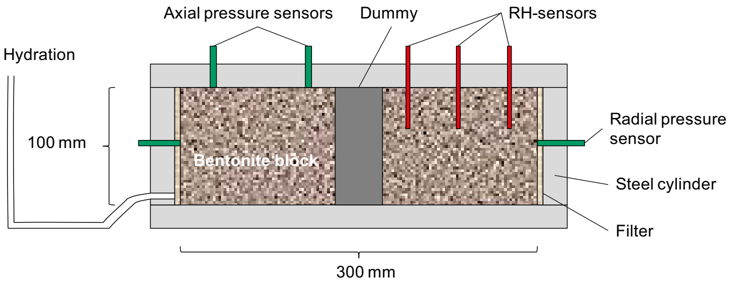
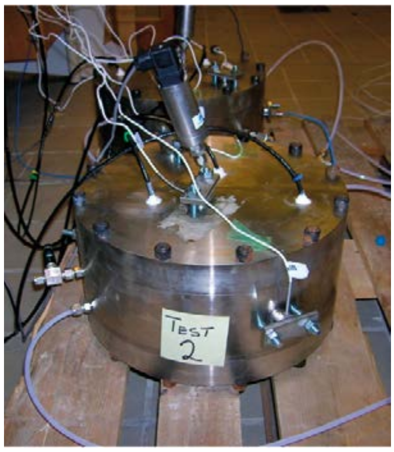


Figure 1-7. *a) "Bentograph" of borehole KO0018G01, and b) interpolated water content measurements (in 72-day intervals) of bentonite installed in borehole KO0017G01 (from Fransson et al. 2017).*

Complementing the BRIE field experiment, a laboratory water-uptake test (WUT) was performed by Clay Technology AB (Vidstrand et al. 2017, Fransson et al. 2017) to provide relevant information on the wetting behaviour of an MX-80 bentonite cylinder that has the same dimensions, density, and initial water content as the bentonite installed in BRIE (Figure 1-8a). In the WUT, water was supplied either freely or limited to a specified amount to a bentonite cylinder with an initial water content of approximately 11.8 %. Cumulative water-uptake (Figure 1-8b) as well as relative humidity and water content were measured during the experiments.



a)



b)

Figure 1-8. *a) Schematic and b) photograph of the BRIE water-uptake test. Water is introduced via the outer cylindrical filter. The 100 mm bentonite block is identical in material to the stack of blocks emplaced in the BRIE in situ experiments (Vidstrand et al. 2017, Fransson et al. 2017).*

Analysing the WUT data was included in Task 8 mainly as a means to gain confidence in the modelling representation and parameterization of bentonite. Given the specific test layout, the experiment provided the bentonite's water-uptake capacity for the bounding case in which water supply from the surrounding environment is not a limiting factor.

1.4 Modelling groups

The modelling groups involved in Task 8 as part of the SKB Task Forces (TF) on Modelling of Groundwater Flow and Transport of Solutes (G) and Engineered Barrier Systems (E) are listed in Table 1-1. With one exception, the modelling groups conducted (or reported on) only a subset of the subtasks. If no final report was submitted, the review was based on draft or interim reports.

1.5 Overview of Task 8

1.5.1 Overall objectives

Task 8 is entitled "*Modelling of the Bentonite Rock Interaction Experiment, BRIE – an interaction between engineered and natural barriers*". The related task description (Vidstrand et al. 2017) uses the title "*Modelling the Interaction between Engineered and Natural Barriers – An Assessment of a Fractured Bedrock Description in the Wetting Process of Bentonite at Deposition Tunnel Scale"*. This report evaluates the outcome of the Task 8 modelling studies against the overall objectives as described by Vidstrand et al. (2017); they are:

- Improved scientific understanding of the exchange of water across the bentonite-rock interface.
- Better predictions of the wetting of the bentonite buffer.
- Better characterisation methods of the canister boreholes.
- Better methods for establishing deposition hole criteria (this aspect was eventually not considered in this Task Force per mutual agreement).

Task 8 aims at improving our understanding of the hydraulic interaction between the rock and partially saturated bentonite on both the scale of an individual deposition hole as well as the scale of a deposition tunnel. (Note that only the smaller of the two scales was investigated in the subtasks evaluated in this report.) This requires developing appropriate conceptual models and simulating the evolution in space and time of key hydrogeological attributes of the bedrock, the bentonite, and across the interface between these two repository system components.

Table 1-1. Organizations participating in SKB Task Force modelling of Task 8.

Modelling groups			Tasks conducted					
Organization	**Country**	**TF**	**A**	**B**	**C**	**D**	**F**	**W**
Gesellschaft für Anlagen- und Reaktorsicherheit gGmbH (GRS)	Germany	G/E		X	X	X	X	X
Japan Atomic Energy Agency (JAEA)	Japan	G		X	X	X	X	X
Korea Atomic Energy Research Institute (KAERI)	Korea	G	X	X	X	X		
Los Alamos National Laboratory (LANL)	USA	G				X		
Nuclear Decommissioning Authority – Amec Foster Wheeler (NDA-AMEC)	UK	E			X	X	X	
Posiva Oy – VTT Technical Research Centre of Finland Ltd. (Posiva-VTT)	Finland	G	X	X	X	X	X	X
Swedish Nuclear Fuel and Waste Management Co. – Computer-aided Fluid Engineering AB – Golder Associates AB (SKB-CFE-Golder)	Sweden	G	X		X	X		X
Swedish Nuclear Fuel and Waste Management Co. – Clay Technology (SKB-Clay Tech)	Sweden	E	X		X	X	X	X
Swedish Nuclear Fuel and Waste Management Co. – Royal Institute of Technology (SKB-KTH)	Sweden	G	X					
Swedish Nuclear Fuel and Waste Management Co. – Stockholm University (SKB-SU)	Sweden	G	X	X	X	X	X	
Technical University of Liberec (TUL)	Czech Republic	E	X			X		X

Supporting the design and analysis of the Bentonite Rock Interaction Experiment (BRIE), which was conducted concurrently with Task 8 at the Äspö Hard Rock Laboratory, is an ancillary objective of Task 8. BRIE consists of several boreholes (drilled in rock of different degrees of fracturing). Some of these boreholes were used to characterize the fractured rock of the test bed. Others were drilled vertically into the floor. These probing holes were hydraulically tested before they were widened to become surrogate deposition holes, which were initially open to inflow, but were subsequently filled with partially saturated bentonite. Total stress, pore water pressure and relative humidity were measured in the bentonite and in the adjacent bedrock. After a suitable time two of the holes were over-cored and the bentonite recovered and analysed mainly for water content distribution.

1.5.2 Subtasks

Task 8 consists of several interlinked subtasks with specific objectives. Some of these subtasks were developed or adjusted during the course of the Task 8 modelling work in response to the availability of supporting data, insights gained during preceding subtasks, as well as progress and special interests stated by the modelling groups.

This report is concerned with the following subtasks:

Task 8A Initial – Scoping calculation

Task 8B TASO – Scoping calculation

Task 8C BRIE – Prediction for central deposition hole

Task 8D a) BRIE – Prediction of inflow and wetting of KO0017G01 and KO0018G01 based on detailed characterisation data

b) Water-uptake test

Task 8F BRIE – The Final Task 8 BRIE Modelling

The following subsections contain a brief summary of the individual tasks; the detailed task description can be found in Vidstrand et al. (2017).

1.5.3 Task 8A: Initial scoping calculations

Modelling the interaction between initially partially saturated bentonite and the surrounding fractured bedrock requires a modelling approach (and associated simulation software) that can appropriately represent the properties and behaviour of both media as water flows through them. The purpose of the initial scoping calculations was:

- To determine means of incorporating bentonite in numerical groundwater flow models.
- To evaluate effects of different implementations of the bedrock-bentonite interface in groundwater flow models.
- To supply guidance to the field experiment on the importance of bedrock fractures.

Task 8A also addressed the key issue of localized water entry through a fracture into the bentonite-filled borehole, and whether this could lead to a heterogeneous hydration of bentonite. The non-uniformity of the hydration is likely to depend on geometry as well as the chosen combination of rock and bentonite hydraulic properties. These combinations were examined through sensitivity analyses, which also helped identify the bounds for which the hydration is predominantly controlled by the bentonite or the bedrock.

Two generic problems were defined based on the overall design of the surrogate deposition hole and the engineered barrier (Figure 1-9a):

Case 1: Two-dimensional axi-symmetric set-up of intact rock (green), bentonite (blue), and a tunnel cross-section. For this case, the rock fracture (purple) should be ignored and replaced with intact rock.

Case 2: Two-dimensional axi-symmetric set-up of intact rock, one rock fracture (purple), bentonite, and a tunnel cross-section.

Details about material properties, initial and boundary conditions, and simulation scenarios can be found in Vidstrand et al. (2017). The system behaviour with and without a fracture was to be represented by the temporal evolution of pressure and/or saturation in the bentonite, rock, and fracture.

1.5.4 Task 8B: TASO Scoping calculations

Task 8B consisted of scoping calculations using a simplified sub-local model of the Äspö Hard Rock Laboratory (HRL), referred to as the TASO tunnel, which is the test bed for BRIE. It required the inclusion of site-specific conditions and addressing the impact of fractured bedrock on inflow into open probing holes and open surrogate deposition holes as well as the re-saturation of a bentonite-filled surrogate deposition hole.

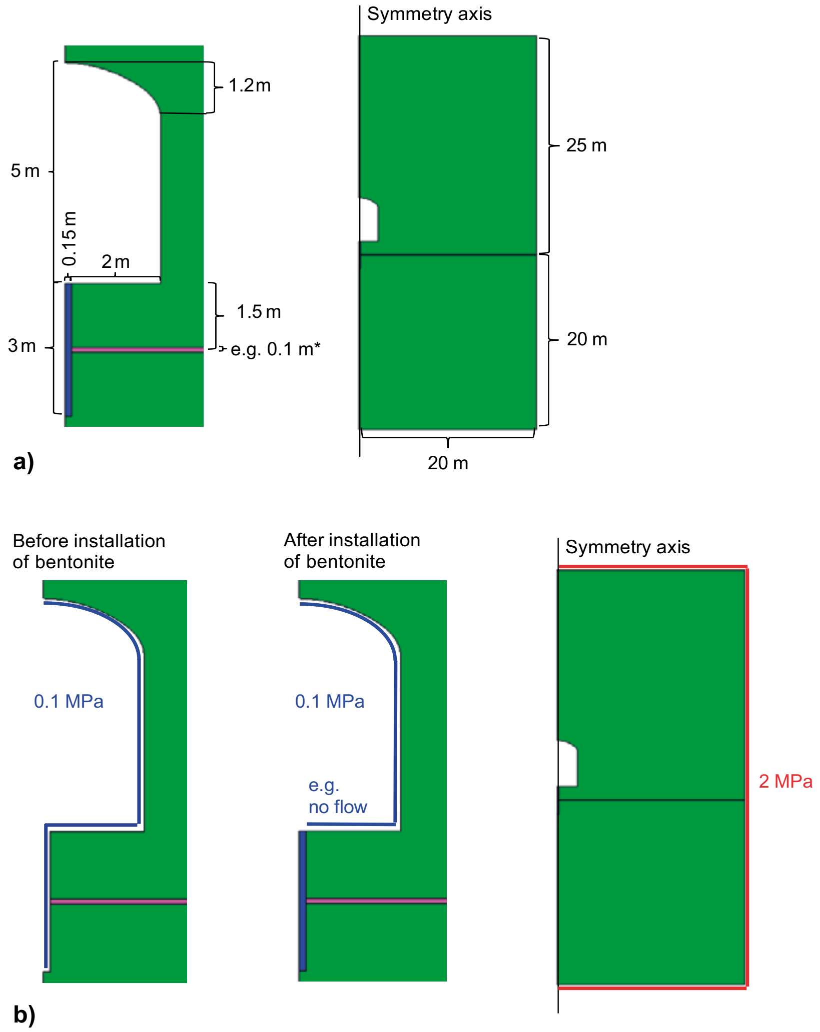


Figure 1-9. *a) Model domain and b) boundary conditions for initial scoping calculations of Task 8A (from Vidstrand et al. 2017).*

The main objectives of this scoping exercise were (Vidstrand et al. 2017):

- To determine means of incorporating partially saturated rock and to examine effects of different concepts and properties
- To evaluate effects of different representations of fractured rock, to examine effects due to contrasts between matrix and fracture properties, and to reveal the significance of fractures
- To evaluate effects of the fracture location along the deposition hole on the resulting wetting of the bentonite
- To evaluate effects of boundary conditions assigned to large cavities
- To provide guidance to BRIE on the importance of bedrock fractures and matrix and where to place monitoring sensors

Figure 1-10 shows the tunnel layout and the proposed model domain (a cube with side lengths of 40 m), along with the pressure distribution calculated using a regional model of the Äspö HRL, from which the boundary conditions for the Task 8B model can be extracted. The geometry of key geological planar features was also provided as part of the task description. Pressure and saturation distributions in the rock and the bentonite were used as reportable performance measures.

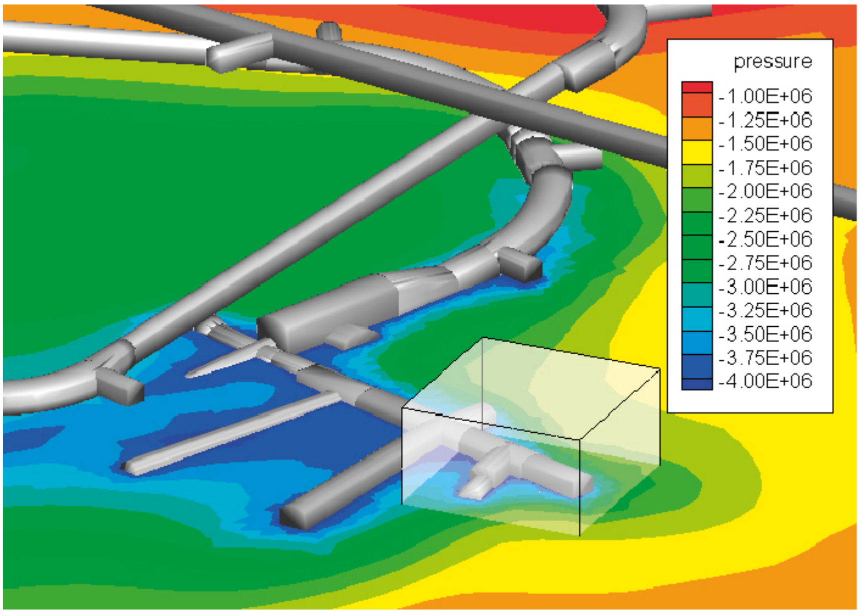


***Figure 1-10.** TASO tunnel, model domain, and pressure distribution calculated by a regional model (from Vidstrand et al. 2017).*

1.5.5 Task 8C: BRIE – Prediction for central surrogate deposition hole

Task 8C consisted of two parts. In the first set of simulations, inflow into an open surrogate deposition hole was predicted based on limited characterization data; in the second set of simulations, the rewetting of the bentonite was predicted. The main objectives were:

Task 8C1

- To predict inflows and inflow characteristics to deposition holes.
- To set up the main features of the TASO site.
- To test the adopted boundary conditions in relation to the site-specific deformation zones.
- To supply guidance to the field experiment on importance of bedrock fractures and matrix and where to place monitoring sensors.

Task 8C2

- To evaluate effects of the fracture locations along the deposition hole on the resulting wetting of the bentonite.
- To serve as a base case for comparison with later results based on more elaborate hydrogeological models.

The predictions of inflow to the boreholes in the TASO tunnel were done for a sub-local Äspö HRL site model domain (similar to that of Task 8B), which included the main geological structures depicted in Figure 1-11.

In addition to the deterministic geologic structures shown in Figure 1-11, statistical information on three fracture sets was provided. Initial and boundary conditions were akin to those of Task 8B.

Unlike Task 8B, measurements of pressure build-up in packed-off, small-diameter (0.076 m) probing holes were available, so were outflow measurements after the holes were opened to atmospheric conditions. Injection tests were also performed, with monitoring of pressure responses in neighbouring holes providing information on connectivity. All these measurements were made available as potential calibration data.

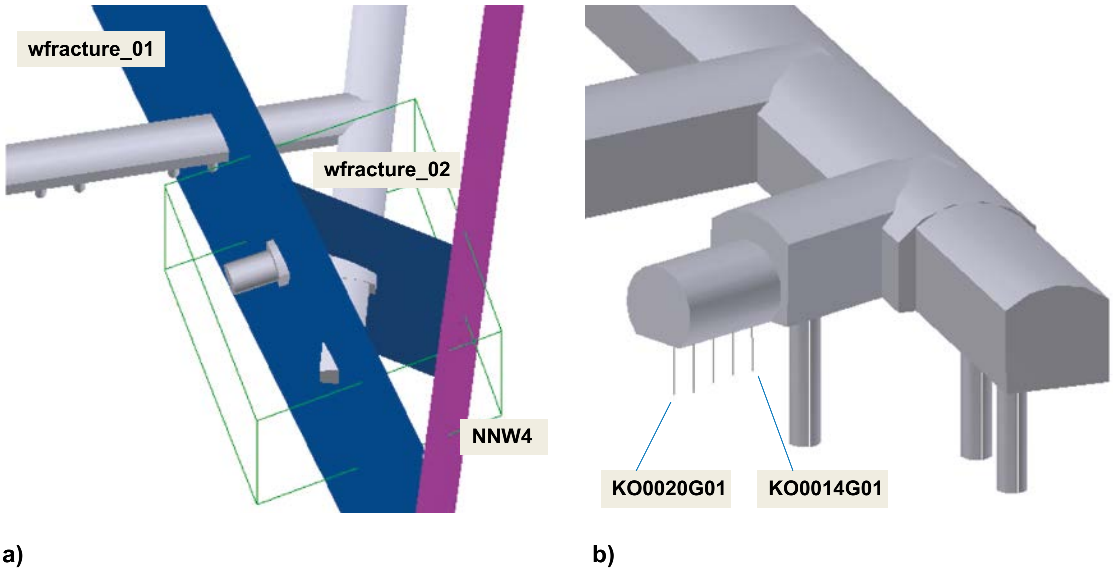


Figure 1-11. *a) TASO tunnel, model domain, and large, deterministic geological structures; b) surrogate deposition holes (from Vidstrand et al. 2017).*

Two of the probing holes were then expanded to a diameter of 0.3 m, which is the configuration for which predictions of inflow to such surrogate deposition holes were made. Finally, bentonite was placed into these holes. The wetting process was simulated, and the associated spatial and temporal wetting patterns along with the pressure evolution within the buffer and the bedrock was predicted.

1.5.6 Task 8D: BRIE – Prediction of inflow and wetting

Task 8D consisted of two subtasks, similar to Task 8C. In the first set of simulations, inflow into an open surrogate deposition hole of diameter 0.3 m was predicted based on more detailed information than in Task 8C, and compared to field observations from BRIE. In the second set of simulations, the wetting of the bentonite was calculated and used as a prediction for the BRIE field experiment. The main objectives were:

Task 8D1

- To calculate inflows and inflow characteristics to two 0.076 m diameter probing boreholes.
- To calculate inflows and inflow characteristics to two 0.3 m diameter open boreholes.
- To compare inflows calculated for probing boreholes with inflows calculated for enlarged 0.3 m boreholes.
- To supply structural model, boundary conditions and initial conditions to the field experiment on the emplaced bentonite packs within the two 0.3 m diameter boreholes.

Task 8D2

- To evaluate effects of the borehole characteristics on bentonite wetting.
- To evaluate effects of heterogeneous fracture flow on bentonite wetting.
- To evaluate effects of heterogeneous matrix properties on bentonite wetting.
- To compare with earlier results which were based on less elaborate hydrogeological models.

The modelling task was similar to that of Task 8C, with additional characterization data available.

1.5.7 Task 8F: BRIE – The final Task 8 BRIE Modelling

Previous subtasks have involved predictive modelling, where results from bentonite wetting were not available to the modellers. Task 8F provided the opportunity to perform concluding simulations by making use of the results documented in the BRIE report (Fransson et al. 2017). The purpose of these final analyses was:

- To discuss the predictive modelling and compare them with experimental results.
- To perform inverse modelling and back-analyses.
- To evaluate the wetting of the bentonite installed in the two boreholes.
- To re-evaluate the initial hypotheses and address sensitivities concerning conceptual issues.

A data set of particular value and interest (specifically regarding model conceptualization, characterization and influence of discrete geologic structures, and bentonite wetting) are the so-called "bentographs", showing traces of bentonite wetting at the outer circumference of the bentonite (see Figure 1-7a), as well as relative humidity and water contents measured within the bentonite (see Figure 1-7b). The modelling activities were similar to those of Tasks 8C2 and 8D2.

1.6 Performance measures

Distinct performance measures were refined in the task descriptions to generate a common set of outputs for comparison between models and with data, and to facilitate succinct reporting and evaluation of the behaviour of the fractured rock-bentonite system. The performance measures were intended to document the model structure, overall simulation results, as well as specific predictions. They generally included the following:

- Visualizations of permeability structure.
- Visualizations of pressure, saturation, and flow fields in the model domain, the immediate vicinity of the surrogate deposition holes, and within the bentonite.
- Visualization of inflow patterns to open deposition holes.
- Predicted evolutions of pore pressure, relative humidity, and saturation at representative points.
- Predicted inflow rates to open surrogate deposition holes.
- Predicted times for rewetting of surrogate bentonite to specific saturation levels.

To reflect uncertainties in the model predictions, ranges of predicted inflows and rewetting times were requested.

In addition to these quantitative performance measures, the modelling groups were encouraged to provide analyses, interpretations, and discussions that support the overall Task 8 objectives.

1.7 Questionnaires on uncertainty

As outlined in Section 1.5.1, the overall objective of Task 8 was to obtain a better understanding of the hydraulic interaction between the near-field bedrock and backfill materials in the repository. The fact that multiple models of the same repository subsystem are available provides a unique opportunity to examine conceptual model uncertainty.

To facilitate a cross-comparison study, a process has been proposed (see Appendix A) that aims at compiling and discussing conceptual model uncertainty within the context of the specific repository subsystem, hydrogeological features, numerical models, and target predictions these models were asked to deliver as part of Task 8.

The modelling groups were asked to respond to a questionnaire that solicited input and descriptions of system understanding, features implemented, as well as explicit and implied assumptions along with an assessment of the validity and uncertainty of these assumptions. In addition, results from the various sensitivity analyses and more general evaluations of the quality of model predictions and their uncertainty were requested.

The survey results were compiled and discussed in a special workshop during the Task Force Meeting #34 in Prague. While the outcome of these discussions will be reported separately in an article that focuses on conceptual model uncertainty, some of the issues raised by the questionnaire were addressed and reported also in the final reports of Task 8, which form the basis for this evaluation.

1.8 Comments on task description

This subsection contains some remarks on the task description (Vidstrand et al. 2017) and the process used to guide the Task 8 modelling work towards the stated objectives.

The task descriptions were developed and released stepwise in a series of documents and revisions; they were eventually combined in Vidstrand et al. (2017). In addition, data files and reports documenting the BRIE experiment (to which Task 8 is linked) were distributed to the modelling groups.

The initial task description of April 2010 outlines the key objectives, describes the BRIE experiment, and provides specifications for Tasks 8A, B, and C (see Section 1.5). Along with descriptions of the problems to be solved by numerical modelling, rather detailed information about certain aspects of the system was provided, including geometries of the model domain, engineered underground structures, and large hydrogeological features, as well as initial and boundary conditions, material properties, and statistical parameters of the fracture network. A list of specific output variables at predefined points in space and time was provided and were to be considered by the modelling groups as the expected, reportable outcome of the modelling studies. This initial Task description was amended and revised multiple times in response to discussions and decisions reached during Task Force meetings, and as new data from BRIE and related interpretations became available. New subtasks were added. The schedule was adjusted accordingly.

The following comments are some general remarks and observations regarding the task description.

- The process of drafting, revising, reviewing, adjusting, and issuing multiple task descriptions provides the flexibility needed to organize modelling studies that are related to a concurrent field experiment.
- The task description partly guided the modelling groups' work, and partly responded to the interests, preferences, accomplishments, and schedules of the modelling teams and the progress of the BRIE experiment.
- Rather detailed specifications were given to the modelling groups regarding certain aspects of the system. Moreover, suggestions were presented regarding properties and features to be included in the model. The choice and level of detail of these descriptions probably had the following impact on the modelling studies:
    - The detailed specifications accelerated model development as many time-consuming data-analysis and model-conceptualization steps were provided and thus eliminated from the modelling groups' workflow.
    - The detailed specifications may have prolonged model development as most of the modelling groups felt compelled to include many (mostly geometrical) details provided in the task description into their models. The relevance of some of these details was not always obvious; some were proven insignificant. Providing a complete set of data in the task description is considered appropriate; however, it might be beneficial to highlight that an extensive data set is provided for completeness only, and that it is the modelling groups' responsibility to interpret and abstract them as part of the model conceptualization process.
    - The detailed specifications may have led the modelling groups to focus on implementation aspects rather than system understanding, conceptualization, and interpretation. The detailed specifications suggested that site-specific predictions were sought, which is in partial contradiction to the stated objectives of gaining more general understanding of the interactions between fractured rock and bentonite.

- Some specifications were very detailed, others incomplete or absent; the level of detail did not always correspond to the relevance of the described feature. As stated above, this is appropriate as it reflects data availability rather than their relevance. The modelling groups could be explicitly encouraged to find and justify the appropriate level of detail, appropriate for the intended use of their models.
- The specifications led the modelling groups to develop similar conceptual models, thus limiting the variety of alternative conceptual models that probably would have been developed if the specifications had been less prescriptive. It is noted, however, that the ensemble of all developed models shows a relatively broad range of conceptual models.
- Features for which no specifications were given tended to be de-emphasized. Specifically, no information about the interface between the fractured rock and the bentonite buffer was provided. This may have been the reason why limited attention was given to the nature, conceptualization, and properties of the interface despite it being one of the study objectives of Task 8.

• The desired interaction between numerical modelling and field experimentation could have been outlined in more detail. The use of numerical models in support of experimental design and data analysis, and the role of field observations and experimental results for system understanding, conceptualization and model validation could have been made more explicit. It may have been beneficial if the task description had discussed the extent to which design calculations, blind predictions, as well as sensitivity, uncertainty, and data-worth analyses could be used in support of BRIE, and how data collected in BRIE could be used for conceptualization, model development, calibration, and validation. While challenging, this interaction between modelling and experimentation could also have been used to better guide the schedule.
• Uncertainty (in data, parameters, conceptualizations, and predictions) could have been made an integral part of the task description.
• The relation between the objectives of the individual subtasks and the overall goals of Task 8 is not clearly articulated. Similarly, the link between expected outcomes and stated objectives is not always evident. As a result, some of the declared task goals were not fully addressed (e.g. the development of better methods for borehole characterization and the establishment of deposition hole criteria was de-emphasized by mutual agreement between SKB and the modelling groups, as the design of the modelling exercises did not clearly indicate that support for these goals was expected).

It is recognized that writing a task description is difficult, as it requires finding a balance between providing adequate guidance and at the same time sufficient leeway to the modelling groups' own approach and interests. Moreover, the subject is scientifically and technically demanding, and the coordination with an on-going field experiment is challenging.

Despite the comments above, the task description documents provided a good roadmap for the Task 8 modelling exercises. The willingness of the Task 8 Technical Committee to adjust the descriptions in response to the needs and preferences of the modelling groups and the BRIE project made it possible to obtain considerable insights into the interaction between the fractured rock and the buffer, and to gain some confidence into the predictability of bentonite re-saturation.

1.9 Scope and structure of review

This report forms part of an independent review of the specifications, execution, and results of Task 8. The review has been carried out by:

• Participating in SKB Task Force workshops and meetings.
• Providing intermediate evaluations during SKB Task Force meetings.
• Organizing special sessions (specifically on uncertainty issues) during SKB Task Force meetings.
• Participating in teleconferences with the Task Force secretariat and Task 8 leadership.
• Reading and commenting on the Task 8 description (see Sections 1.5 and 1.8).

- Reviewing drafts of the final project reports, which included providing specific review comments to the individual modelling groups.
- Evaluating the responses to the questionnaire concerning conceptual model uncertainty (see Section 1.7).
- Interacting with individual modelling teams.

The performed modelling work is mainly documented in the modelling groups' final project reports. Most of these reports include extensive and detailed descriptions of the models developed for each subtask, the corresponding results, and some interpretations and additional analyses. Only summaries of this work can be provided as part of this evaluation report. The purpose of these short descriptions is simply to document the main approach, assumptions, results and conclusions of the individual modelling groups as a basis for the subsequent evaluation. Moreover, as shown in Table 1-1, there is no complete and consistent set of studies conducted by all the participating modelling groups that could be used for an overall evaluation and comprehensive cross-comparison analysis (an attempt at an initial comparative analysis is described in Chapter 4). The structure, length, and content of each subsection thus vary considerably.

The modelling groups used different terminology to describe identical or similar processes and components. No attempt was made to standardize the terminology in this evaluation report. Specifically, Section2 (which summarizes the work of the modelling groups) uses the terms chosen by the modelling groups.

The report is structured as follows:

- Chapter summarizes the work performed by each modelling group.
- Chapter 3 summarizes the key comments from the review of the modelling groups' final project reports.
- Chapter 4 attempts to synthesize the findings obtain by the modelling groups for each of the subtasks.
- Chapter 5 provides an overall evaluation and concludes with some recommendations.

The documentation of the formal review resolution process is considered part of this evaluation.

This evaluation is supplemented by a separate study dedicated to conceptual model uncertainty (Finsterle et al. 2018). Appendix A contains a document describing the approach of this comparative analysis and an associated questionnaire distributed to the modelling groups (see also Chapter 4).

Appendix B contains a list of scientific journal articles and other relevant publications produced by the modelling groups based on their work on Task 8.

Appendix C contains a glossary of terms used in this report. Most of these terms emerged or were defined during the discussions among the Task 8 modelling groups.

2 Summary of modelling work

2.1 Modelling group: GRS

2.1.1 Introduction

The modelling work performed by the Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH, Braunschweig, Germany, is documented in Kröhn (2017, 2018).

The report discusses Tasks 8A-D and Task 8F. GRS opted to not participate in Task 8A, as the underlying concept of the task description was considered incompatible with the proposed approach to simulate bentonite re-saturation. The GRS model of Task 8B only considered the fractured rock, i.e. bentonite rewetting was not simulated. In Task 8C1, the widening of two probing holes was not considered. Task 8C2 revealed that the assumption of free water access at the boundary is a limitation of the VIPER code. The code's capabilities were then expanded. While no rewetting simulations under water-limited conditions were performed for Task 8C2, such simulations were conducted as part of subsequent subtasks. GRS also modelled Clay Technology's laboratory water-uptake experiment.

2.1.2 General modelling approach

The general modelling approach pursued by GRS is to decouple groundwater flow in the bedrock from bentonite re-saturation. To link the two subsystems, the predicted outflows from the rock were provided as boundary conditions for the EBS model. The choice of this sequential approach, which does not account for feedback mechanisms between the natural and engineered barrier systems, appears to be driven by the fact that the groundwater flow code d^3f (Schneider 2012) only handles saturated flow through fractured-porous media; the code is thus not suitable to represent re-saturation processes in the bentonite.

A hybrid representation of the geologic formation was used to simulate groundwater flow through the fractured rock. Large fractures were deterministically implemented as discrete, planar, homogeneous geologic structures according to the specifications in the task description. Small fractures (characterised in statistical terms in the task description) were not explicitly modelled, but were considered part of a homogeneous background rock continuum with a permeability that is higher than that of the intact rock matrix. This effective permeability was first estimated from fracture data, but later determined through model calibration. Some intermediate size fractures (referred to as "user-defined fractures") were inserted as needed to reproduce the variability and rates of inflow into open probing and surrogate deposition holes. Finally, all underground openings (tunnels, boreholes) were accurately reproduced in the model and surrounded by zones with altered hydraulic properties to capture skin effects. All simulations of groundwater flow in the geosphere were transient simulations run to steady state.

The code VIPER (Kröhn 2011) is used to simulate water-uptake and re-saturation of the bentonite. VIPER considers one-dimensional, axisymmetric wetting assuming unrestricted water access, and includes vapour diffusion in the pore space, water diffusion in interlamellar space, and instantaneous exchange of water between these two spaces using an adsorption isotherm (Figure 2-1). The limiting assumption of unrestricted water access at the boundary was removed during the course of the project (Kröhn 2017; Appendix F), allowing bounding calculations to be performed also for flow-restricted imbibition from the background rock.

2.1.3 Task 8B: TASO – Scoping calculations

Model setup

GRS developed a model for Task 8B that includes seven deterministic geologic structures implemented discretely as planar fractures (Figure 2-2). These large features intersect the boundaries of the model domain, where pressure boundary conditions were specified according to the task description. Slight discrepancies in the location of these geologic structures relative to those used in the regional model of the Äspö Hard Rock Laboratory (which provided the boundary conditions) as well as assumptions about the connectivity of these features beyond the model domain led to local pressure distributions and fluxes in these structures that were considered biased, thus influencing the predictions of inflows to tunnels and boreholes.

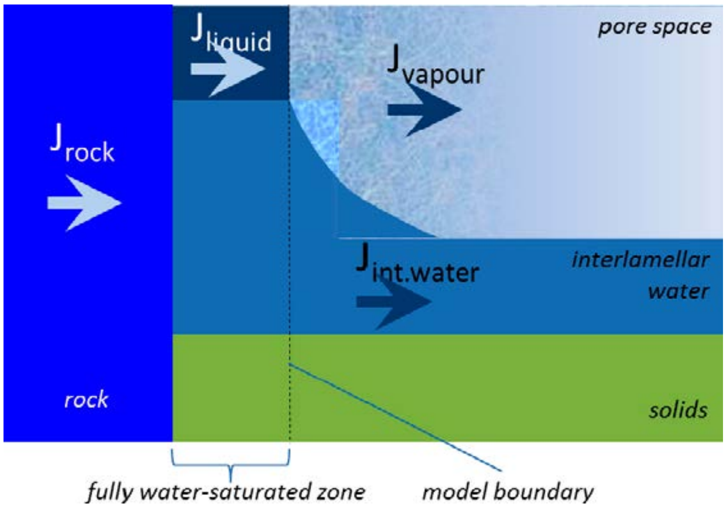


Figure 2-1. *Conceptual model implemented in VIPER code for unrestricted water supply (from Kröhn 2011; Appendix F).*

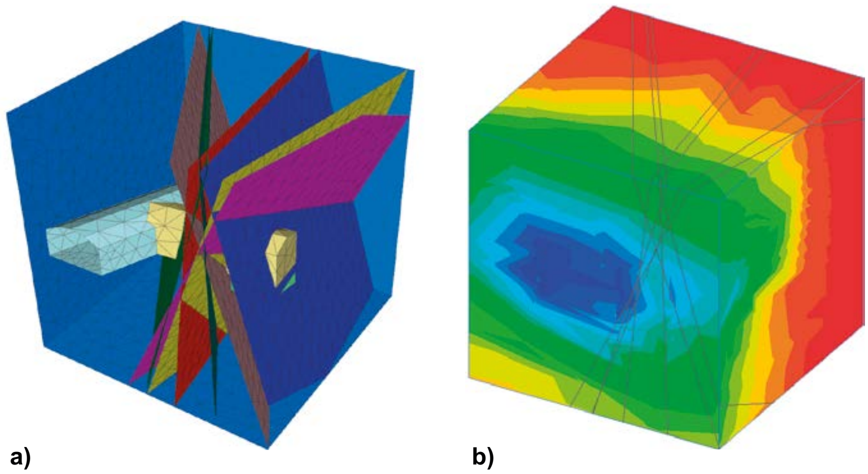


Figure 2-2. *GRS model developed for Task 8B; a) discretization; b) pressure at model boundaries (from Kröhn 2017).*

Results

Pressure distributions (Figure 2-3), velocity fields (Figure 2-4), and inflows into tunnels and boreholes (with a total rate of approximately 180 grams per second) were calculated for steady-state saturated flow conditions. While no comparison to measured data was sought in Task 8B, the predicted inflows to the tunnels seemed large compared to later estimates, and inflows to open holes exhibited stronger variability than those obtained with a model that uses uniform background rock properties. The impact of the large geologic structures on pressure distribution and related flow rates was recognized, but considered biased due to potential inconsistencies in the boundary conditions.

Conclusions

The d^3f code was found to be a suitable tool for simulating saturated steady-state groundwater flow in a formation with fractures that are represented by discrete features as well as effective continuum properties. A calibration step is needed to determine the hydraulic properties of the fractured formation. Moreover, other conceptual assumptions (uniform properties; boundary pressures) specified in the task description led to results that appear strongly biased, reducing the predictive capabilities of the model.

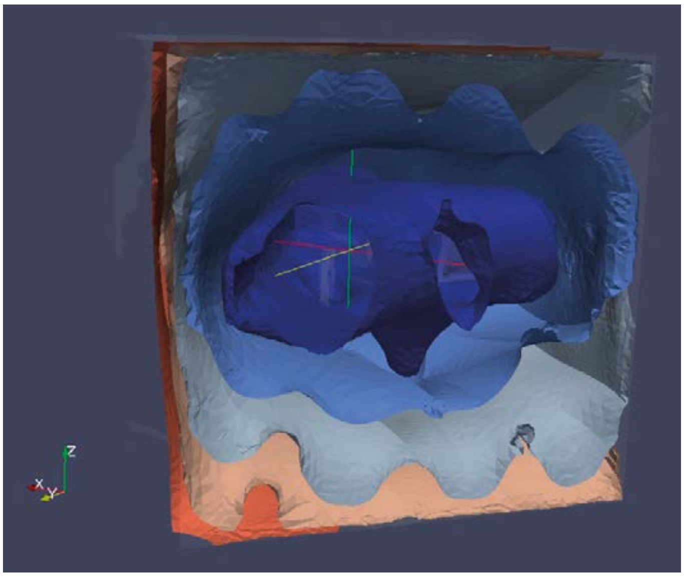
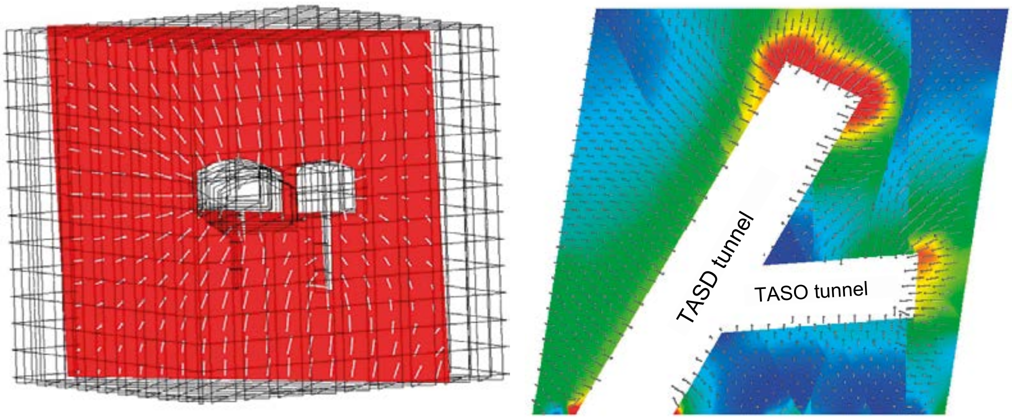


Figure 2-3. *Steady-state pressure distribution, showing influence of discrete features (from Kröhn 2017).*



a) **b)**

Figure 2-4. *Steady-state flow-velocity distribution in a) a fracture, b) background rock (from Kröhn 2017).*

2.1.4 Task 8C1: BRIE – Prediction of inflow to probing holes

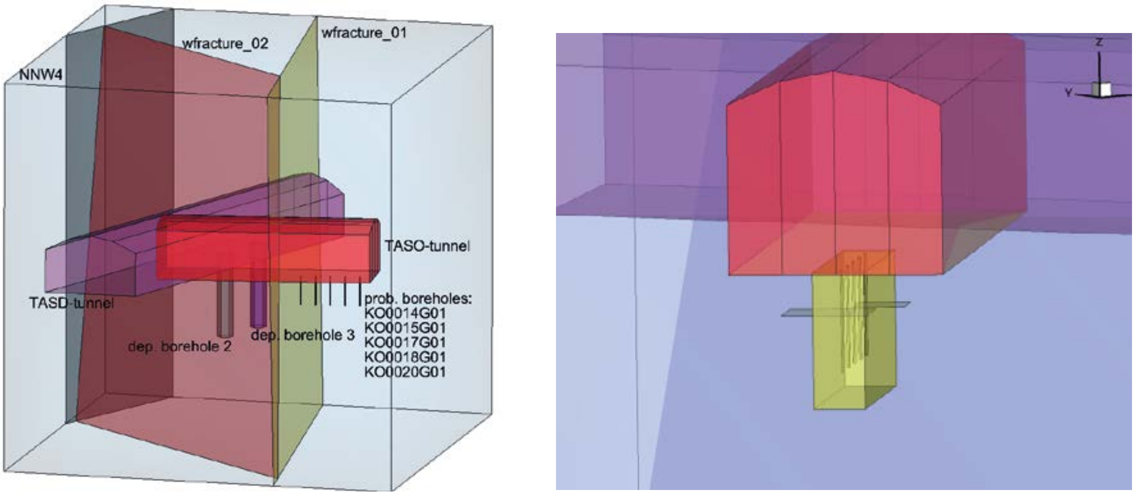
Model setup

The same modelling approach was followed for Task 8C1 as described for Task 8B, except for the following adjustments (Figure 2-5):

- Only three deterministic geologic structures were implemented.
- A low-permeability zone representing undisturbed rock was specified around deposition holes.
- Two discrete user-defined fractures intersecting high-inflow locations were introduced as to better match the observed flow distribution.

Results

Using measurements of inflow into the TASO tunnel and the five surrogate probing boreholes, the permeabilities of the background rock, the skin zone, and one of the two user-defined fractures were adjusted to calibrate the model by simulating different configurations of open and closed probing holes. A substantial increase in background and skin-zone permeability as well as an adjustment of the user-defined fracture intersecting borehole KO0014G01 was needed to match all the measured inflow data within a factor of four.



a) b)

Figure 2-5. *GRS model developed for Task 8C1; a) location and geometry of underground openings and large discrete features; b) skin zone (yellow) around probing boreholes and user-defined fractures (grey) (from Kröhn 2017).*

Conclusions

The following conclusions were drawn from the modelling and calibration exercise of Task 8C1:

- The three large fractures do not influence the inflows into the probing holes, but affect the total inflow to the TASO tunnel, which was well matched.
- Inflow into the probing holes depends on background permeability and the permeability of the assumed fractures that connect the background fracture network with the borehole.
- The effective background permeability of the rock mass, which reflects the matrix and smaller-scale fracture network, is substantially higher than estimates of intact rock permeability.
- It is difficult to capture local variations in inflow to probing holes; intermediate-sized fractures appear to be relevant; however, the data show limited connectivity between the probing holes, even though they are only 1.5 m apart.
- The pressure gradient around the TASO tunnel affects the driving force for inflow; the proximity of the openings to the model boundaries may have a systematic effect on simulation results.
- The stochastic nature of small-scale fractures as well as uncertainty in the conceptual model describing the processes, features, and potential sources of water entering boreholes prevents the model from making deterministic predictions; predictions of average inflows, however, are considered feasible.
- A much higher model and data resolution is required to be able to predict variations in inflow to closely spaced probing holes
- Multiple alternative conceptual models could explain the observed flow distribution; the use of a single, specific model as a predictive tool is thus questioned.

2.1.5 Task 8C2: BRIE – Prediction of bentonite wetting

Model setup

Wetting of the bentonite is simulated using a one-dimensional, radial re-saturation model based on the VIPER code (Kröhn 2011), assuming unrestricted water supply from the formation.

Results

The water content profiles during bentonite re-saturation are shown in Figure 2-6. Imbibition from the outer boundary, which is held at a constant relative humidity of 100 %, resulted in flow rates that are substantially smaller than what could be provided through a fracture (i.e. the assumption of unrestricted water supply is considered appropriate), but is higher than predicted inflows from the background rock.

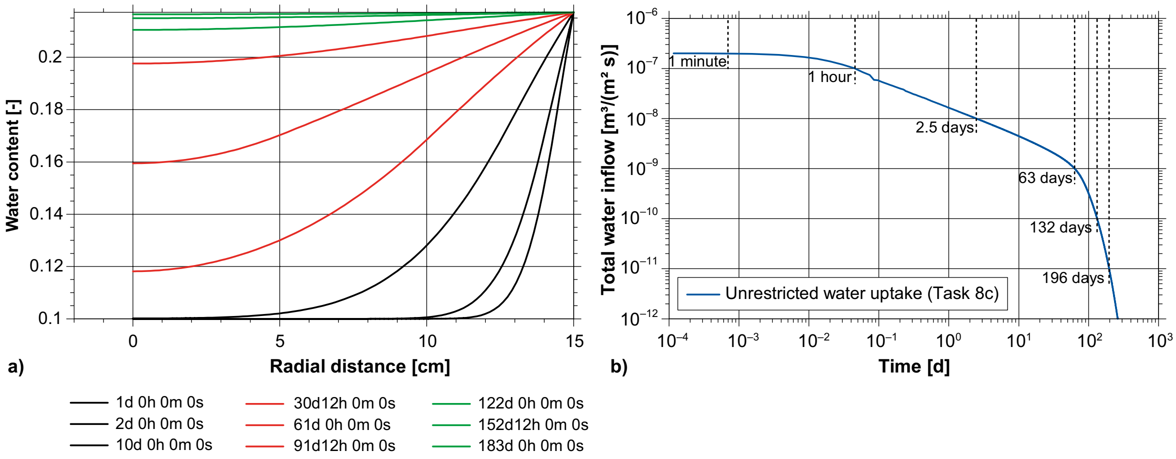


Figure 2-6. *Simulated bentonite re-saturation assuming unrestricted water access; a) water content profiles; b) imbibition rates (from Kröhn 2017).*

Conclusions

The following conclusions were drawn from the Task 8C2 simulation of water-uptake by the bentonite:

- Re-saturation is independent of the details of groundwater flow in the rock as long as the water supply from the formation exceeds the rate of water-uptake by the bentonite
- Water demand by the bentonite may be greater than water supply to an open borehole from the formation, which may indicate a limitation in both the VIPER code and the chosen coupling approach.
- Both regimes (unrestricted and restricted water supply) are considered important, as they refer to expected conditions of deposition holes that are dominated by background rock or fracture flow.

2.1.6 Task 8D1: BRIE – Prediction of inflow to two surrogate deposition holes

Model setup

The same modelling approach was followed as described for Task 8C1, except for the following adjustments (Figure 2-7):

- The user-defined fractures were replaced by skin zones around each underground opening.
- Twenty-three boreholes were explicitly represented in the model.

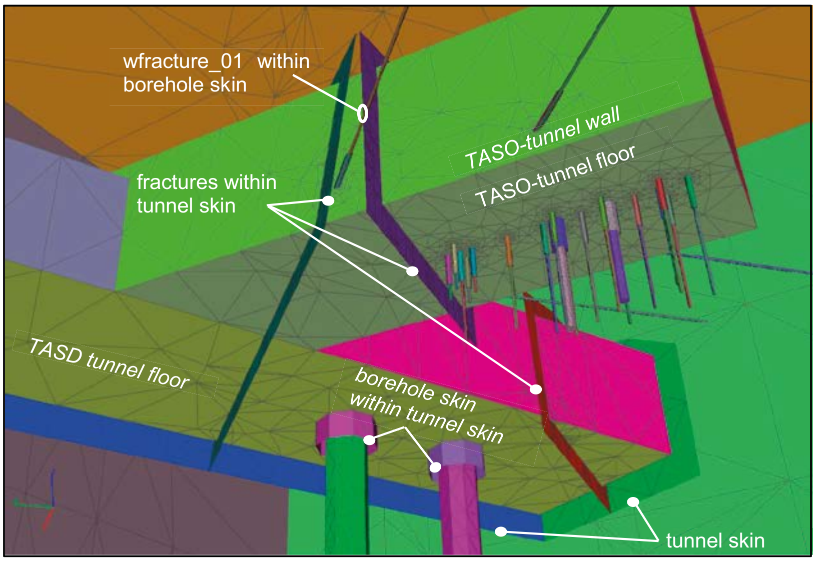


Figure 2-7. *Model developed for Task 8D1, showing tunnel and borehole skin zones (from Kröhn 2017).*

Results

Sensitivity analyses were performed to examine the impact of the skin zone on the pressure field and inflow rates. Using properties from the calibrated model from Task 8C1, predictions of inflow to open boreholes were made that matched the measured data reasonably well. Inflow to borehole KO0011G01 was not well reproduced, which was attributed to a systematic error in the extent of one of the large fractures and its proximity to the model boundaries. Simulating different configurations showed only minor borehole interference.

Conclusions

The following conclusions were drawn from the Task 8D1 modelling exercise:

- The effective permeability of the background rock (10^{-17} m^2) exceeds the value of the undisturbed matrix by about three orders of magnitude, reflecting the well-connected network of smaller fractures.
- The skin permeability around the tunnels is one order of magnitude lower than the effective background rock permeability; the skin permeability around the boreholes is two orders of magnitude lower than the effective background rock permeability, possibly accounting for degassing effects; the permeability of fractures within the skin is one order of magnitude lower than fracture permeability outside the skin.
- Predictions based on a homogeneous, deterministic model fail to reproduce the variability observed in closely spaced boreholes.
- Not all discrepancies between the model and data could be resolved.

2.1.7 Task 8D2: BRIE – Prediction of bentonite wetting and water-uptake test

Model setup

The VIPER code was enhanced (Kröhn 2017; Appendix F) so it can handle specified flux (i.e. Neumann) boundary conditions for the simulation of restricted water supply at the bedrock-bentonite interface. The revised code was used to simulate Clay Technology's water-uptake test. The general model setup is similar to that of Task 8C2, with the exception that the presence of the central tube was accounted for.

The following scenarios were considered:

- Inflow concentrated to a single fracture of aperture 0.1 mm (unrestricted water supply as encountered in borehole KO0017G01).
- Inflow over a 1-m long borehole section (restricted water supply as encountered in borehole KO0018G01).
- Conditions reflecting the Clay Technology water-uptake test (unrestricted water supply).

Results

The discussion of pressure and flow rate distributions focused on the influence of the assumed skin zones around geotechnical openings, with trends that are consistent with expectation and in overall good agreement with field observations; no further calibration was deemed necessary. The larger-scale pressure trends (e.g. gradients towards the face of the TASO tunnel) were also evaluated.

Rewetting simulations with restricted and unrestricted water supply resulted in saturation times (to 95 %) of 240 and 535 days, respectively (Figure 2-8b). Given the model assumptions, the results are insensitive to the calculation of geosphere water supply as long as water access can be considered unrestricted. Under restricted flow conditions, however, saturation times are strongly inversely correlated to the water supply rate.

The Clay Technology water-uptake test was well reproduced (Figure 2-9) after adjustment of the interlayer tortuosity.

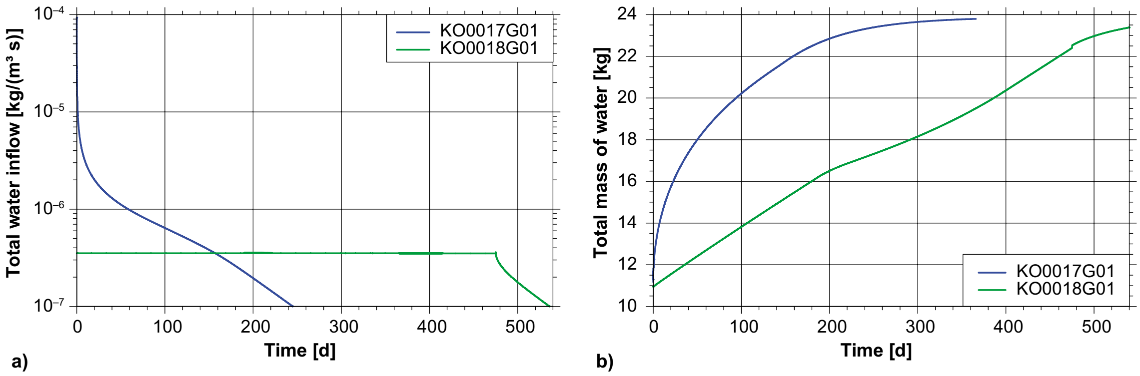


Figure 2-8. *Simulated radial imbibition test under restricted and unrestricted water supply conditions; a) imbibition rate; b) cumulative imbibition (from Kröhn 2017).*

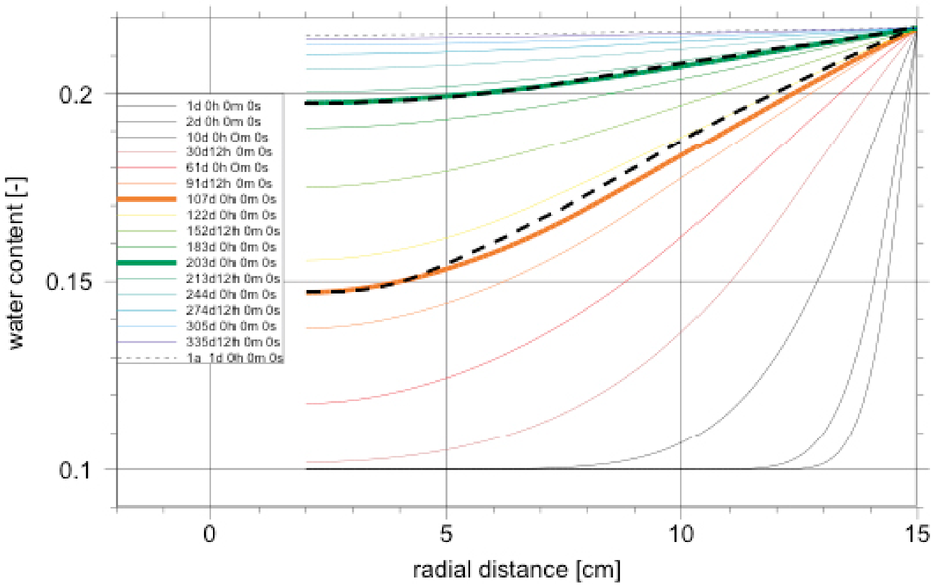


Figure 2-9. *Prediction of water content distribution in the water-uptake test; measured data shown as black dashed line (from Kröhn 2017).*

Conclusions

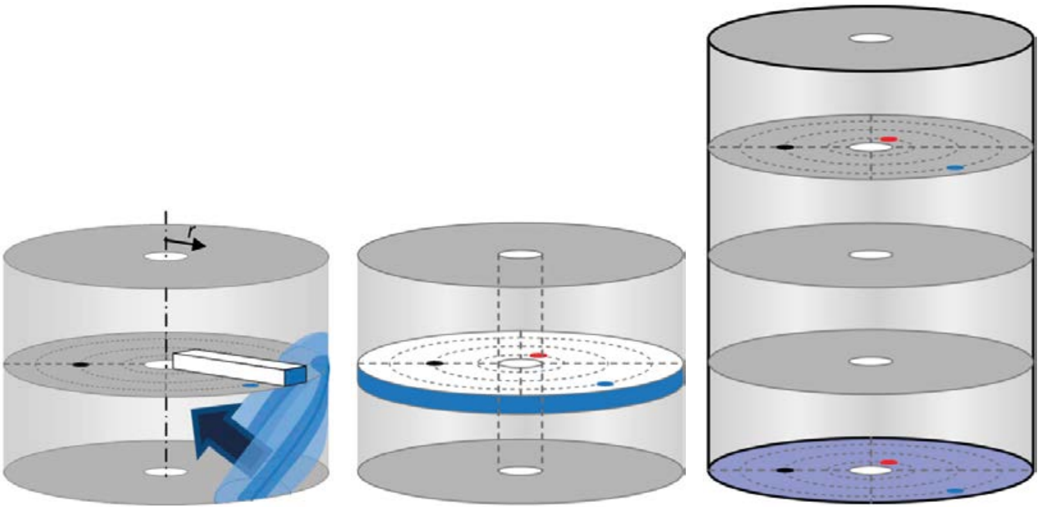
The following conclusions were drawn from the Task 8D2 simulations of bentonite re-saturation and water-uptake test:

- Water supply from the formation may be the limiting factor for bentonite re-saturation, thus affecting wetting time.
- The one-dimensional model used for the analysis may underestimate wetting times.
- The laboratory water-uptake test was well reproduced after an adjustment of tortuosity.

2.1.8 Task 8F: BRIE – Post-test data analysis

Model setup

Focusing on bentonite wetting under relatively dry and wet conditions, models based on different scenarios (restricted vs. unrestricted water supply, respectively) were developed in an attempt to reproduce and explain the moisture distribution observed in the dismantled bentonite blocks. A rather detailed examination of the data, sensor locations, and features preceded the numerical analysis. Events such as the unintentional flooding of the central tube and vertical water migration were also discussed to understand unexpected or complex sensor responses. The resulting model conceptualizations are depicted in Figure 2-10. Various alternatives were also examined.



a) b) c)

Figure 2-10. 3D reconstruction of water-uptake a) from water-conducting fractures, b) from the background rock, and c) by axial water migration (from Kröhn 2017).

Results

Comparisons of calculated and measured relative humidity in wet sections indicated that the assumption of unrestricted water-uptake from fractures appears appropriate, and the conceptual model is capable of reproducing the data collected in the immediate vicinity of the fracture. The intricate distribution within the entire bentonite cross section, however, is not reproducible with this simplified submodel.

For the dry sections, the maximum water supply from the background rock is adjusted to match the data. However, a similar response can also be induced by axial water migration.

Conclusions

The simplified geometry, processes, and boundary conditions implemented in VIPER appear appropriate for capturing the behaviour of certain subsections of the bentonite. Interpretations of sensor behaviour outside these limited zones remain, however, inconclusive. To reproduce small-scale wetting structures, it is essential to accurately capture and implement features and events that were not observed or included in the earlier prediction models. Initial and boundary conditions are influential as well.

The analysis of bounding cases using different wetting scenarios suggests that water inflow from fractures followed by water redistribution within the bentonite are the dominant processes governing bentonite wetting. Water inflow from the background rock is comparatively small.

2.1.9 Concluding statements

GRS reached the following conclusions about the Task 8 modelling exercise:

- Task 8 and specifically the calibration of the model increased the understanding of groundwater flow in fractured rock and its impact on the prediction of bentonite re-saturation.
- Inflow into deposition holes is not significantly affected by the proximity of large water-bearing structures, unless they are directly intersecting the borehole.
- Sub-networks and intermediate-sized fractures are important; however, they are too small for deterministic inclusion, but too big for stochastic treatment.
- Small fractures considerably contribute to the effective permeability of the background rock continuum between the large water-bearing structures.
- Variability in measured inflows cannot be reproduced with the current model, unless local, discrete features are introduced.

- The stochastic nature of the fracture network precludes a deterministic prediction of water inflow into deposition holes.
- Bentonite wetting may occur under restricted or unrestricted water supply from the formation, which affects behaviour and wetting times.
- The bentonite material properties seem adequately characterized for the simulation of rewetting using the VIPER code, with confidence gained by the successful prediction and reproduction of data from the water-uptake test.
- The modelling suffers from considerable conceptual and parametric uncertainties:
  - Potentially systematic errors exist in prescribed model boundary conditions as well as the location and extent of large geologic structures.
  - Hydraulic properties estimated by calibration are highly uncertain due to non-uniqueness.
  - Observed changes in flow conditions lack understanding of underlying reasons and mechanisms.
- It is recommended to:
  - Increase model resolution or to add heterogeneity to the background permeability field to better reproduce observed variability in inflow, even though such an extension may not be justified given conceptual uncertainties.
  - Extend VIPER to include 3D effects as they affected the moisture distribution in the bentonite.
  - Perform probabilistic predictions rather than aiming for deterministic predictions.
  - Increase understanding of features and processes that lead to a skin zone with reduced hydraulic conductivity.

In its final comments, GRS acknowledges the inherent difficulty of predicting flow in a bedrock with fractures on multiple scales. Deterministic predictions are considered infeasible. Stochastic analyses are considered a meaningful approach to obtain estimates of the number of qualified boreholes on the repository scale. However, the approach requires extensive characterization data on multiple scales and covering the entire repository area. Nevertheless, the quality of actual deposition holes needs to be assessed individually.

GRS proposes to develop a catalogue of outflow situations as a basis for a series of bentonite re-saturation simulations. Finally, robust process understanding is considered essential as a basis for any reliable model prediction.

2.2 Modelling group: JAEA

2.2.1 Introduction

The Task 8 modelling work performed by Japan Atomic Energy Agency (JAEA) is documented in Sawada et al. (2019). JAEA did not participate in Task 8A.

2.2.2 General modelling approach

The general modelling approach pursued by JAEA is to decouple groundwater flow in the bedrock and bentonite re-saturation. A discrete fracture network (DFN) model was used to simulate saturated groundwater flow in the fractured bedrock using the code FracMan/MAFIC (Dershowitz et al. 2007, Miller et al. 2001); background rock flow is ignored. A separate code, Thames, capable of simulating coupled thermal-hydraulic-mechanical processes based on the Richards equation, is used to model bentonite re-saturation. The two codes are coupled using two utility programs, MTOT (MAFIC to Thames) and TTOM (Thames to MAFIC), transferring flow rates or heads from the fracture traces of the DFN boundary to the bentonite, and head values from the bentonite back to fracture nodes, respectively. However, negative pressures caused by suction of the bentonite are not transferred to the boundary condition of MAFIC; MAFIC uses atmospheric pressures at the interface, and a maximum flow rate and a discrete head of 5 m was added to stabilize boundary conditions. This scheme (Figure 2-11) partly accounts for feedback mechanisms between the two systems in a time-lagged fashion. The initial state represents steady-state conditions of flow to the open deposition hole. Moreover, at each time step, flow in the fracture network is presumed steady.

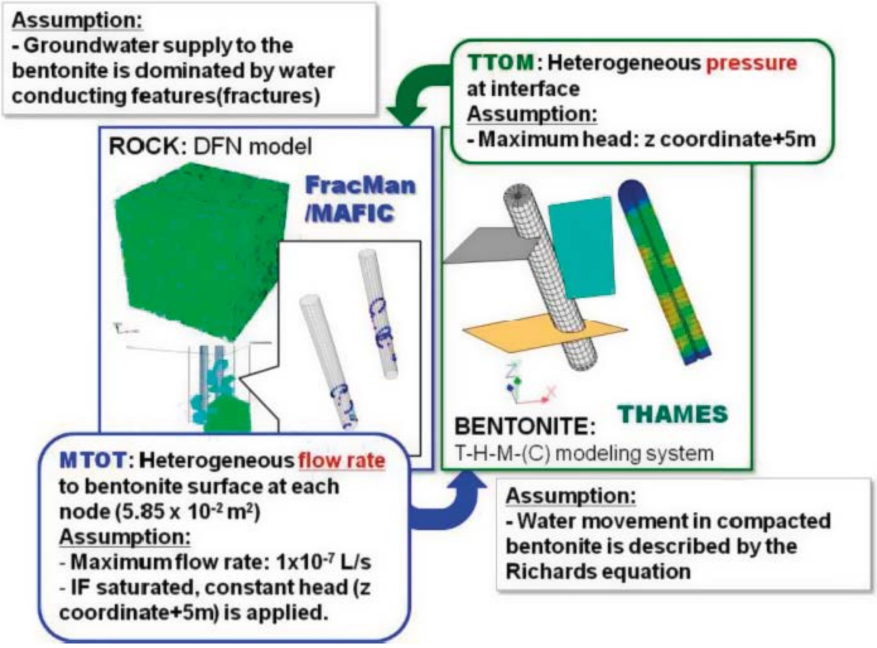


Figure 2-11. Conceptual illustration of a simulation system coupling FracMan/MAFIC and Thames with two interface utility programs, MTOT and TTOM (from Sawada et al. 2019).

2.2.3 Task 8B

Model setup

Three of the large discrete geologic structures specified in the task description were represented in the Task 8B model, consistent with the prescriptions for Tasks 8C and 8D. A hypothetical, horizontal fracture of 5 m radius is also included. No stochastic fracture network is considered, i.e. inflow to the bentonite is limited to a single fracture, which is supplied with water from the three large structures, which are connected to constant head boundaries (see Figure 2-12).

Results

The flux provided through the single (hypothetical) fracture to the bentonite is small, and because it is the only inflow point, it would take over 100 years to re-saturate the bentonite (Figure 2-13). Sensitivity analyses were performed with respect to fracture transmissivity and TTOM's damping factor, showing no impact on final wetting time.

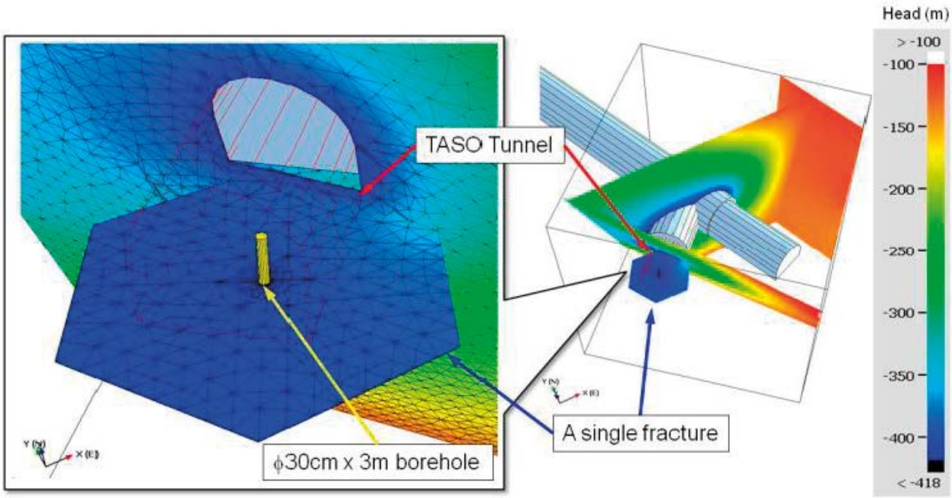


Figure 2-12. Simulated head distribution around a hypothetical single fracture under steady-state conditions with atmospheric pressure specified at the 0.3 m diameter borehole (from Sawada et al. 2019).

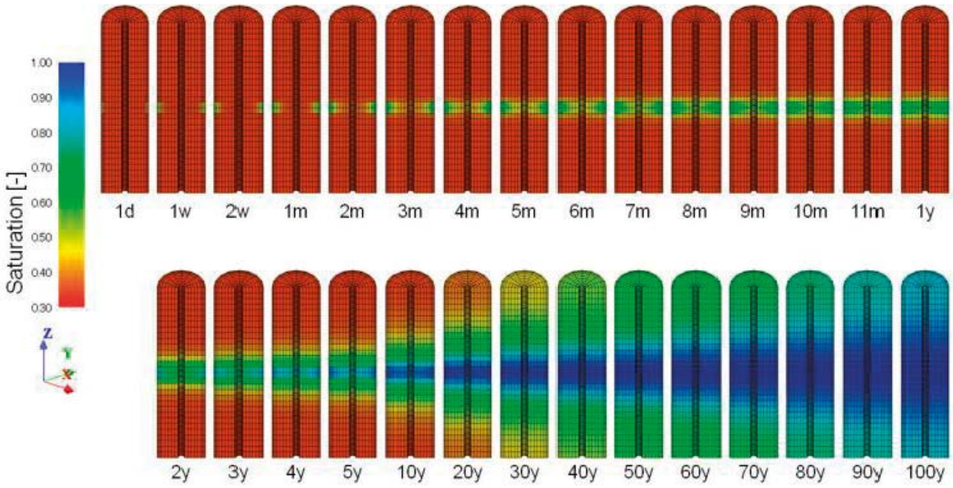


Figure 2-13. *Saturation distribution after installing bentonite into 0.3 m diameter borehole (from Sawada et al. 2019).*

Conclusions

The following conclusions were drawn from the Task 8B modelling:

- The coupling scheme developed to link groundwater flow through a fracture network and water-uptake by the bentonite buffer was demonstrated to provide reasonable results
- The saturation time at the bentonite surface is controlled by availability of groundwater in fractures connecting to the bentonite
- Groundwater flow rate through the interface is controlled by the groundwater diffusion behaviour in the bentonite after it is saturated at the bentonite surface

2.2.4 Task 8C

Model setup

In addition to the three discrete, water-bearing features, a stochastic discrete fracture network model (DFN) consisting of three fracture sets was generated (Figure 2-14). All fractures were considered water conducting, with transmissivities related to fracture length. Fractures smaller than 0.6 m length in the outer model region were removed. The background rock was assumed impermeable. Five realizations of the DFN were examined.

Results

A comparison of the simulated inflows from the five DFN realizations with the measured values indicated that the overall DFN permeability is too high. There is considerable variability (by approximately two orders of magnitude) in the predicted outflows between individual realizations. While only two of the five boreholes showed measureable inflows, the DFN predicted inflows into all boreholes, with (on average) similar rates, i.e. the spatial variability was underestimated.

To better match the observed data, the model was adjusted by a) reducing its overall permeability, b) introducing a "skin" zone near the model boundaries, c) reducing the boundary head value, d) changing the location and transmissivity of one of the large geologic structures, and e) constraining the fracture network characteristics near the boreholes. The conditioning of the DFN to known fractures locations in the five boreholes is illustrated in Figure 2-15.

Results from a single DFN realization were chosen for the simulation of bentonite wetting. The resulting non-uniform water imbibition and bentonite saturation patterns are shown in Figure 2-16.

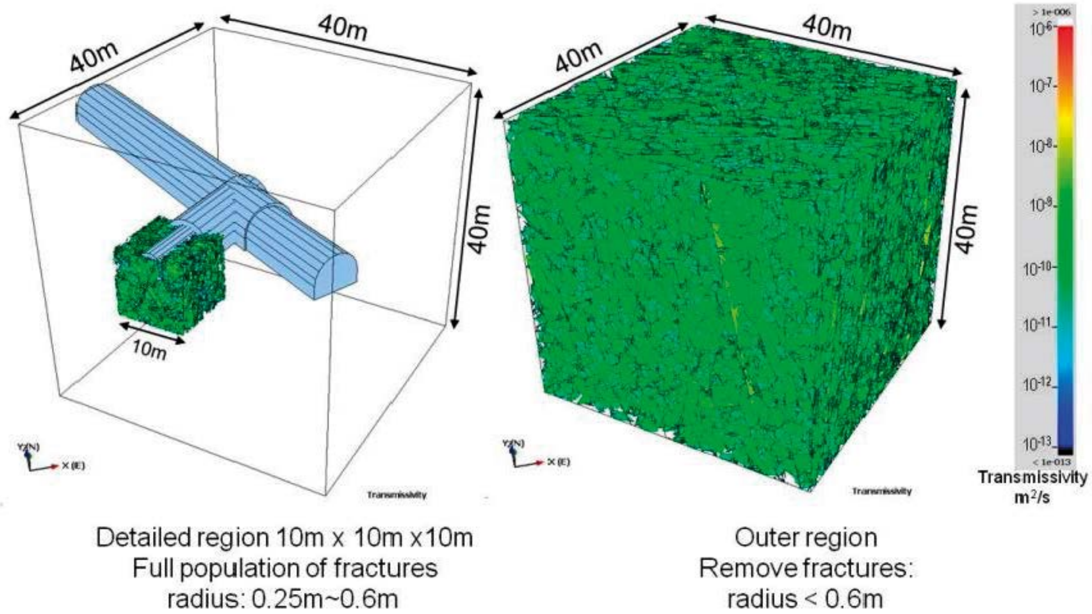


Figure 2-14. *Example of the stochastic background discrete fracture network, generated by FracMan (from Sawada et al. 2019).*

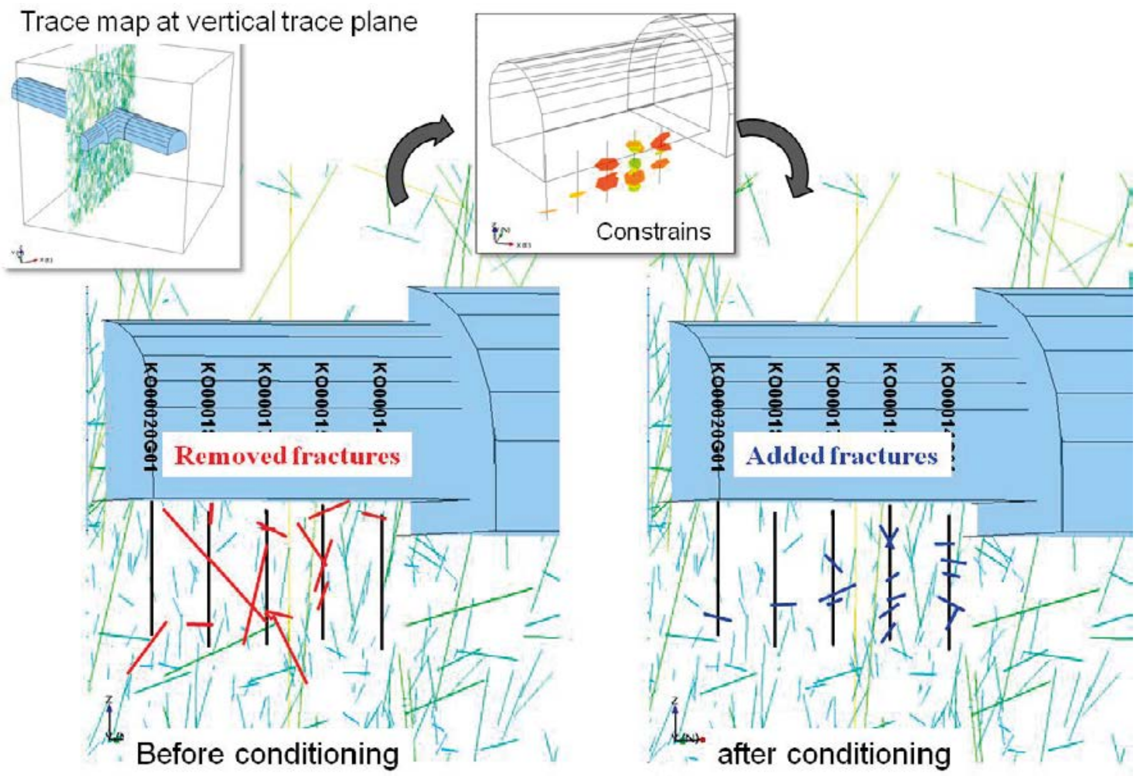


Figure 2-15. *Conceptual illustration of method of the fracture conditioning to specified fracture mapping data (from Sawada et al. 2019).*

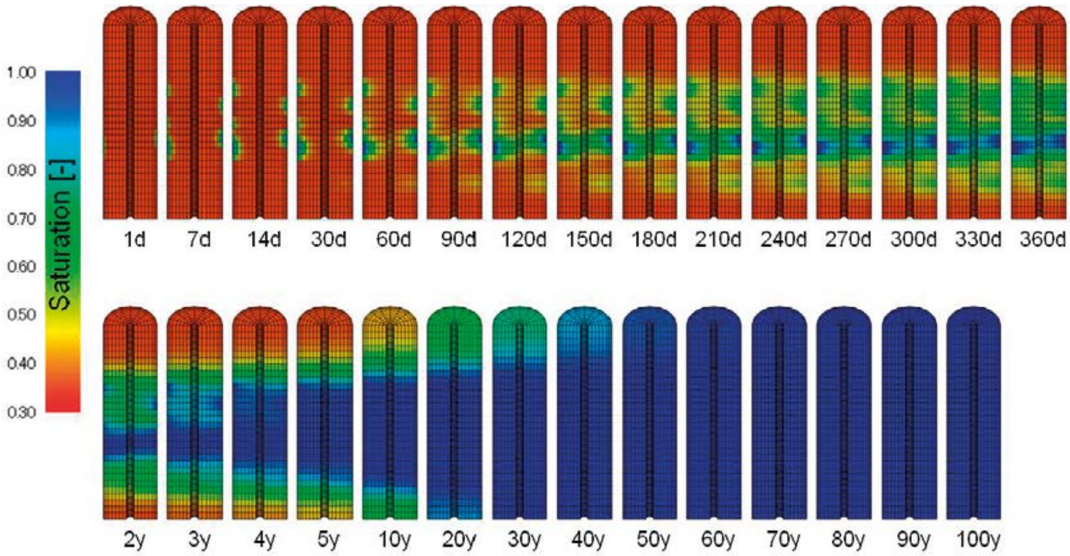


Figure 2-16. *Simulated saturation distribution in bentonite during wetting of surrogate deposition hole KO00017G01 with fracture conditioning (from Sawada et al. 2019).*

Conclusions

JAEA drew the following conclusions from the Task 8C modelling study:

- Different DFN realizations led to wide variability in predicted flow rates and heads at a given point; nevertheless, none of the realizations captured the fact that no inflow was observed in three out of the five boreholes.
- Observed rates and pressure heads could be matched by either reducing transmissivity for all fractures, or by locally conditioning the DFN to fracture traces observed in the boreholes.
- A highly heterogeneous pressure and saturation propagation during bentonite wetting was obtained by coupling the results from the groundwater flow simulation in the DFN to the bentonite re-saturation model.
- Heterogeneous wetting patterns in the bentonite were persistent for at least 10 years.
- The number of discrete inflow points providing groundwater from the fractures to the bentonite and the transmissivity of these fractures control the propagation rate of pressure and saturation in the bentonite column.

2.2.5 Task 8D

Model setup

The modelling approach from Task 8C was used as a basis for the Task 8D model setup. Additional information about borehole flow capacity observed at boreholes KO0014G01, KO0015G01, KO0017G01, KO0018G01 and KO0020G01 was used to constrain the DFN. Transmissivities of fractures intersecting the probing holes were estimated from flow capacity data. The calibration approach is schematically shown in Figure 2-17. The initial saturation of the bentonite was also adjusted.

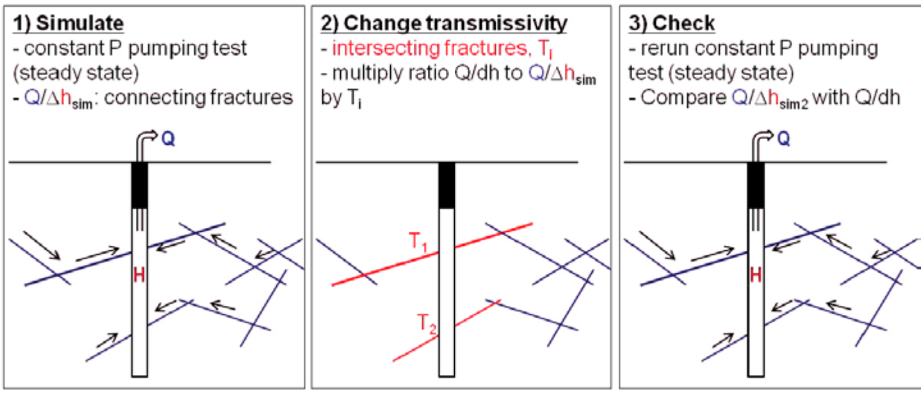


Figure 2-17. *Conceptual illustration for calibrating specific capacity around the five probing holes (from Sawada et al. 2019).*

Results

Multiple scenarios were simulated in addition to the base case to examine the impact of transmissivity changes, fracture conditioning, and different stochastic realizations of the DFN. Alternative boundary conditions and the impact of adding artificial fractures were also examined.

The predicted inflow patterns remained largely unchanged despite the use of additional characterization data. In particular, the base-case scenario significantly over-predicted inflows, motivating the sensitivity case with reduced transmissivity. The variability among the stochastic realizations remained large despite the conditioning and calibration process.

The general wetting behaviour of the bentonite, which is controlled by the fracture pattern at the interface, did not change substantially. However, wetting times changed slightly due to the calibration of the specific capacities of the intersecting fractures.

Conclusions

The wide variability in flow rates and heads among the stochastic realizations persisted, even though the specific capacities around the five probing holes were constrained. Despite considerable adjustments in local transmissivities (estimated by matching capacity data), the impact on bentonite wetting behaviour remained relatively small. Location and hydraulic properties of the water-conducting fractures intersecting the boreholes might be enough to predict bentonite wetting.

2.2.6 Task 8F

Model setup

The same system of the numerical codes as used for the previous tasks were applied to the stochastic DFN, which was updated by correcting the orientation of the water-conducting fractures observed in boreholes KO0017G01 and KO0018G01, and by recalibrating the correlation parameter between transmissivity and fracture size (Figure 2-18). All fracture traces mapped on walls of the five probing boreholes were used to condition the DFN; their transmissivities were adjusted as well to fit measured data (Figure 2-19). Fractures below a certain transmissivity were removed from the DFN to increase computational speed.

One thousand realizations of the stochastic DFN were simulated and compared to measured data to select six realizations for the analysis of bentonite wetting and for visual comparison with the features seen on the "bentograph".

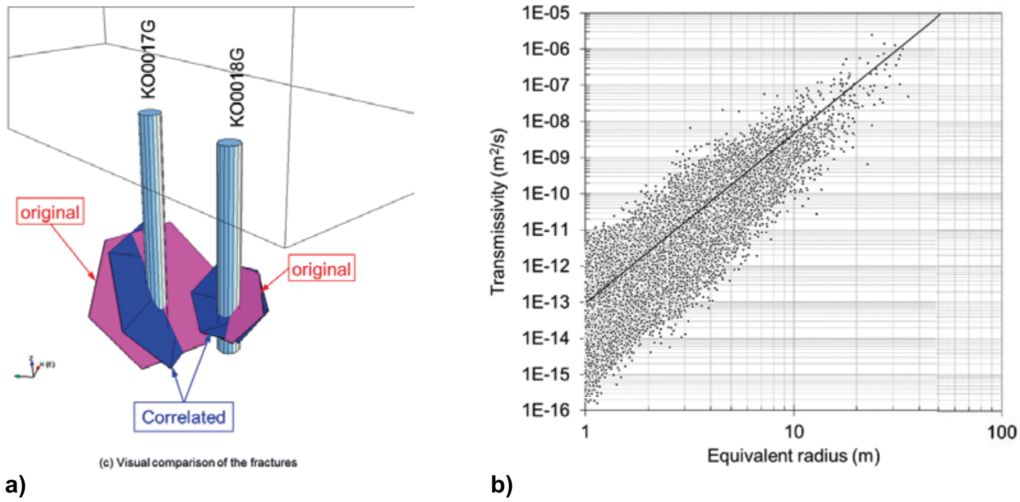


Figure 2-18. *a) Orientation correction of the deterministically defined water conducting fractures, and b) correlation between fracture radius and transmissivity (from Sawada et al. 2019).*

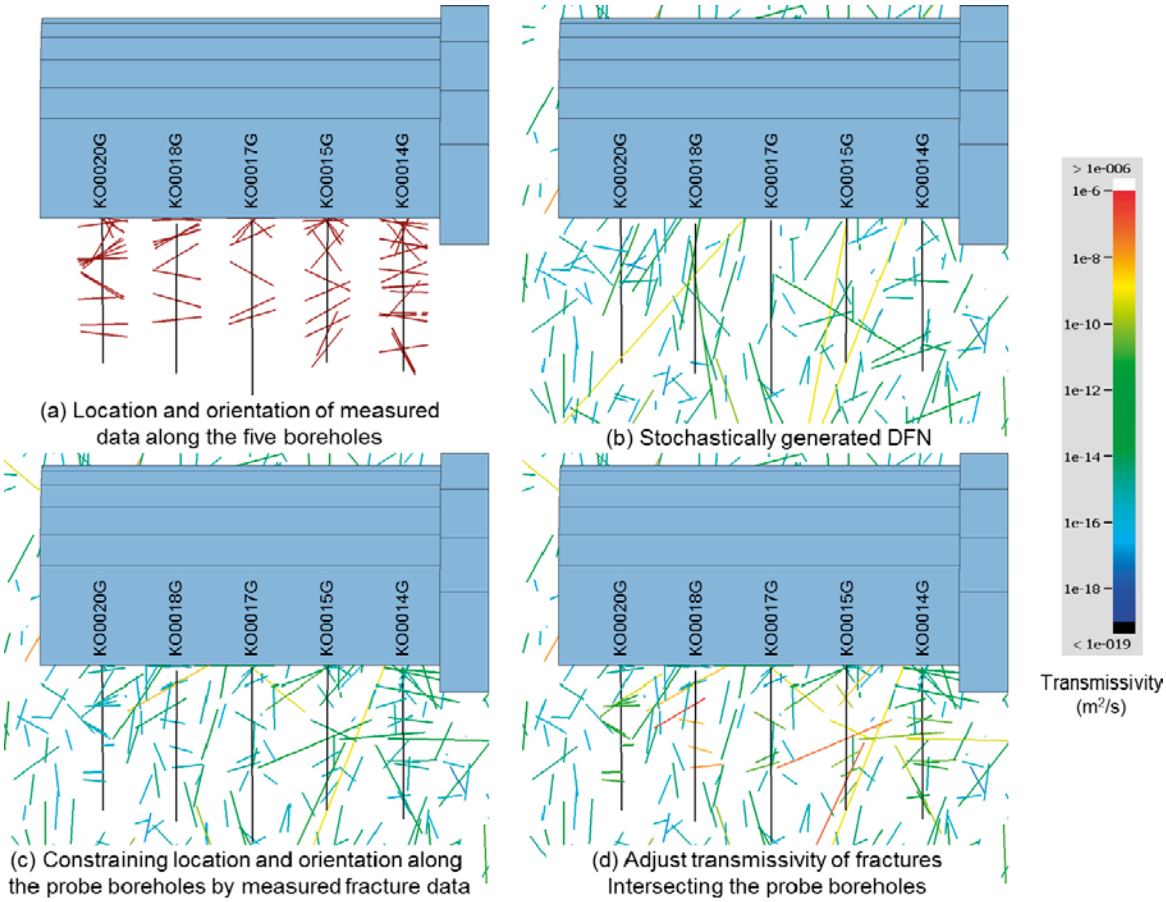


Figure 2-19. *Constraining fracture location and orientation, and adjusting transmissivity of fractures intersecting the probing boreholes (from Sawada et al. 2019).*

Results

The inclusion of data from BRIE into the revised model yielded a transmissivity distribution that is substantially different from that used in the previous subtasks (Figure 2-20). The six realizations used for the analysis of bentonite wetting matched observed pressures and inflows into the five open probing holes reasonably well. However, as illustrated in Figure 2-21, the wetting pattern of the six best-performing realizations led to substantially different wetting patterns despite the conditioning of some of the fractures intersecting the borehole; many of the calculated wetting patterns did not reproduce the observed bentograph wetting patterns very well. This insight also applies to the comparison of calculated and measured relative humidity profiles (Figure 2-22), and water content (Figure 2-23). Despite these early-time differences, most of the realizations predicted complete bentonite saturation within 100 years (Figure 2-24).

Conclusions

In summary, JAEA's FracMan-Thames DFN/Bentonite wetting simulation approach and the assumption of fracture-dominated wetting appears to be able to provide a reasonable approximation to the observed heterogeneous wetting behaviour of BRIE. The location, orientation, transmissivity (flow capacity), and hydraulic connectivity of fractures intersecting the bentonite column have been shown to be the key parameters to model the heterogeneous wetting behaviour in bentonite. The geologically mapped fracture data along the boreholes was shown to be useful to constrain the stochastic DFN model to reproduce the locations of bentonite wetting. However, the hydraulic connectivity and permeability of these mapped fractures are very uncertain. Based on the findings as described above, it is suggested that a systematic investigation at pilot holes, including both geological mapping of the fractures and also testing of the hydraulic properties of the low permeable fractures, is required to predict the observed heterogeneous wetting behaviour in bentonite.

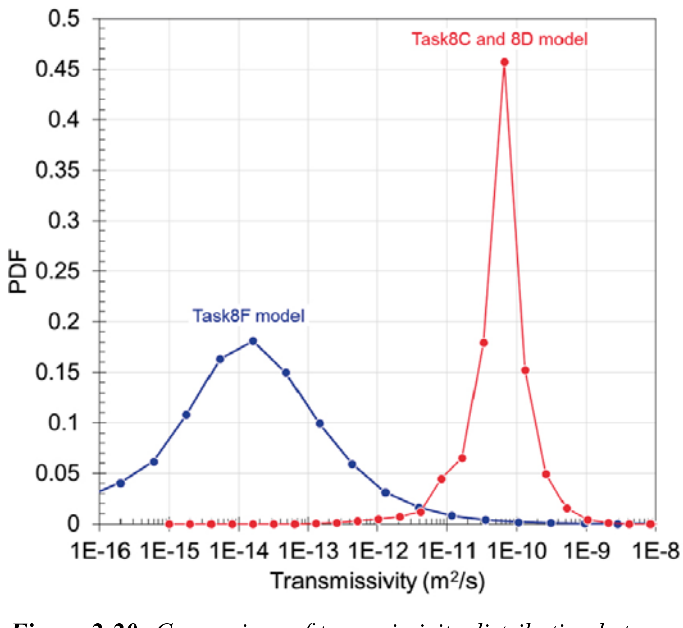


Figure 2-20. *Comparison of transmissivity distribution between Task 8C and 8D model and Task 8F model (from Sawada et al. 2019).*

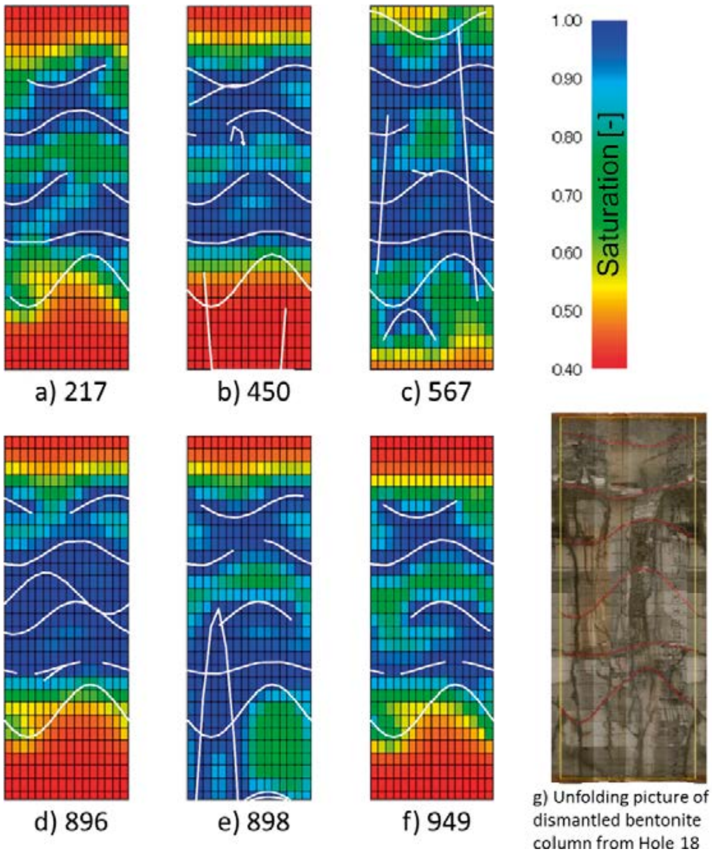


Figure 2-21. *Simulated saturation distribution at the surface of bentonite column after 510 days for twelve DFN realizations a)–f), compared to wetting traces of dismantled bentonite column from Hole 18 g) (from Sawada et al. 2019).*

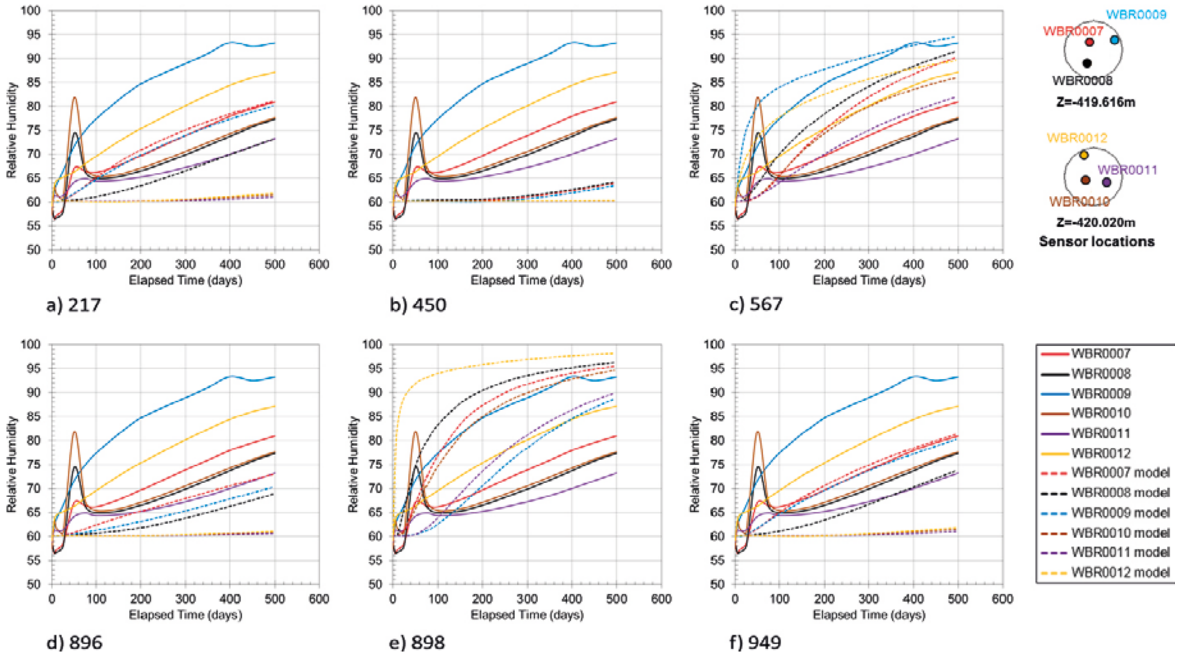


Figure 2-22. *Comparison of simulated relative humidity at six sensor locations with measured data at Hole 18 for six realizations (from Sawada et al. 2019).*

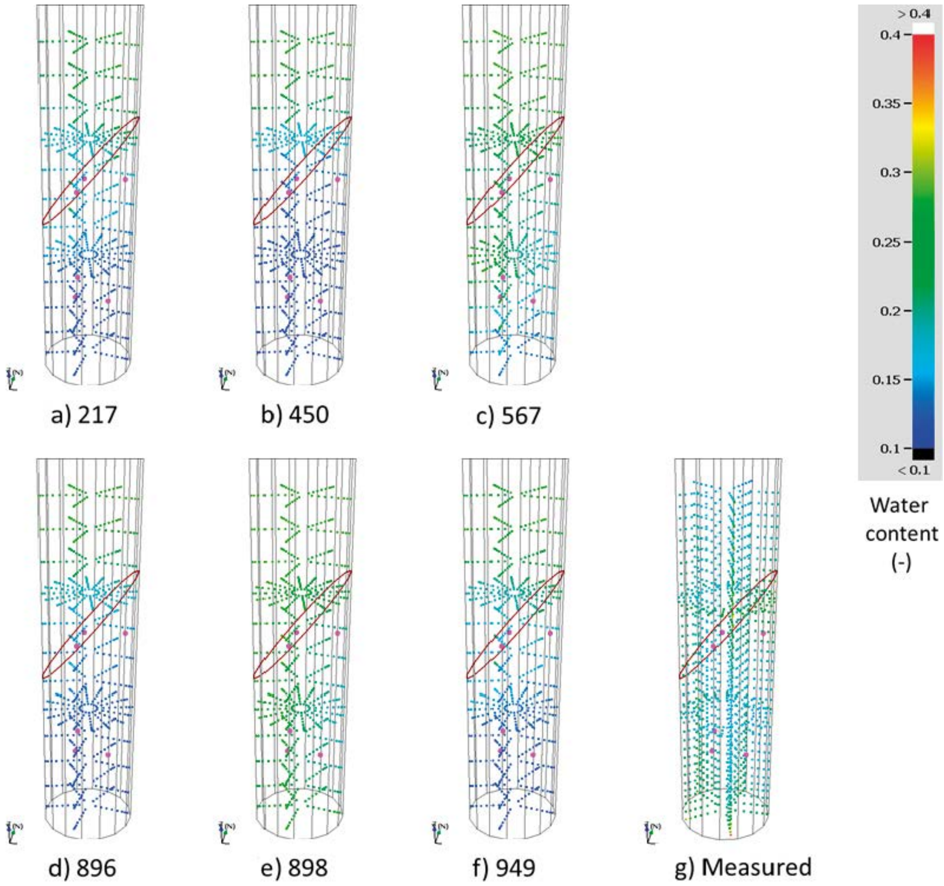


Figure 2-23. *Comparison of simulated water content at the lower part of bentonite column for the six realizations (a) through f)) with g) measured data dismantled from Hole 18 (from Sawada et al. 2019).*

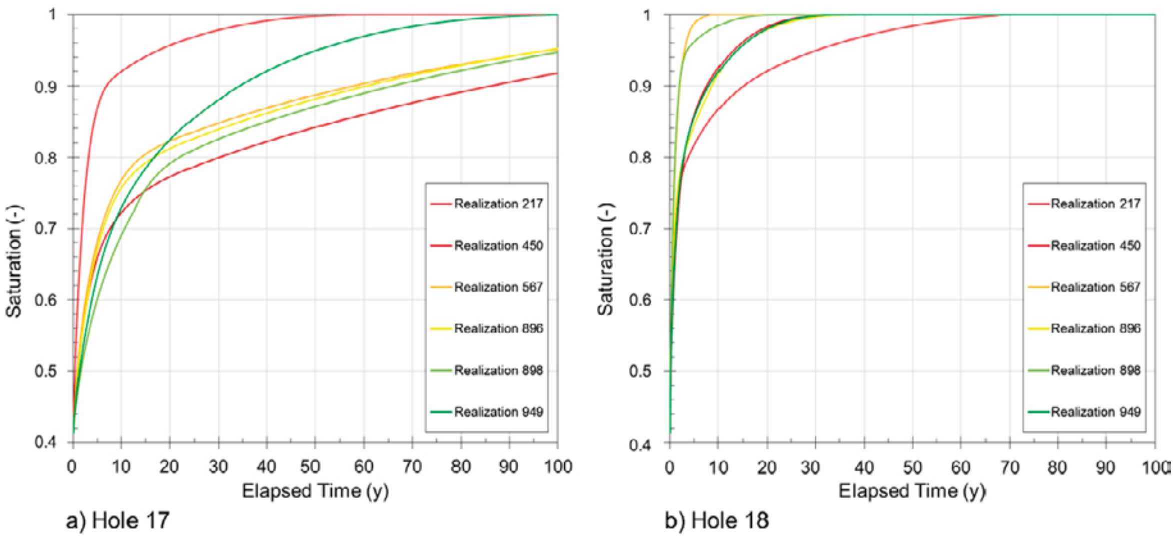


Figure 2-24. *Evolution of saturation of whole bentonite columns for six realizations (from Sawada et al. 2019).*

2.2.7 Water-uptake test

Model setup

The water-uptake test was modelled with Thames using an axis symmetrical model. The initial water saturation of 42 % corresponds to an initial suction of 89.9 MPa. The initial water filling of the outer slot (1mm of clearance between bentonite block and test cylinder) was taken into account by applying water-saturated conditions in the outer 5 mm of the model. The liquid pressure at the outer boundary was kept constant at 0.1 MPa. Figure 2-25 shows the simulation results, which are generally in good agreement with the measured data from the WUT.

2.2.8 Concluding statements

JAEA reached the following conclusions about the Task 8 modelling exercise:

- JAEA‘s DFN model is based on the assumption that the discrete geologic structures dominate the delivery of groundwater to the bentonite columns, i.e. no permeable background rock mass was implemented.
- An iterative coupling between a DFN model (FracMan/MAFIC) and a thermo-hydro-mechanical coupling code for continuous porous media (Thames) was developed and demonstrated to be able to simulate the supply of groundwater through the interconnected fracture network as well as bentonite saturation.
- Stochastic realizations of the DFN model caused wide variability of simulated flow rates to the open holes, even if constrained to the observed fracture locations and the measured specific capacity. The prediction of flowing points and flow rates along the boreholes thus remains a challenge.
- However, knowing the location and hydraulic properties of the water-conducting fractures intersecting the deposition holes may be sufficient to predict bentonite wetting.
- By coupling DFN models to simulations of unsaturated flow in the bentonite, the heterogeneous propagation of groundwater from a limited number of flow points (fractures) could be reproduced.
- The fracture locations and orientations seen in the bentograph are generally consistent with the fracture statistics used to generate the DFN. This indicates that most of the geologically mapped fractures have the potential to provide groundwater to the bentonite even if their permeability is lower than the detection limit of the hydraulic investigation.
- The simulated flow rate and pressure from the 1 000 realizations vary over a wide range; the distributions cover the range of measured values.
- In general, Thames provided a good match to BRIE observations of heterogeneous wetting behaviour in the bentonite column emplaced in boreholes 17 and 18 for twelve select DFN realizations that matched pressures and flow rates reasonably well. Further conditioning was needed to obtain an improved match to the measured heterogeneous bentonite wetting. This indicates that the hydraulic connectivity and transmissivity of the intersecting fractures significantly influence the heterogeneous wetting distribution of the bentonite columns.
- It is suggested that a systematic investigation at pilot holes, which includes geological mapping of the fractures and testing of the hydraulic properties of the low permeable fractures, is required to predict the observed heterogeneous wetting behaviour in bentonite.

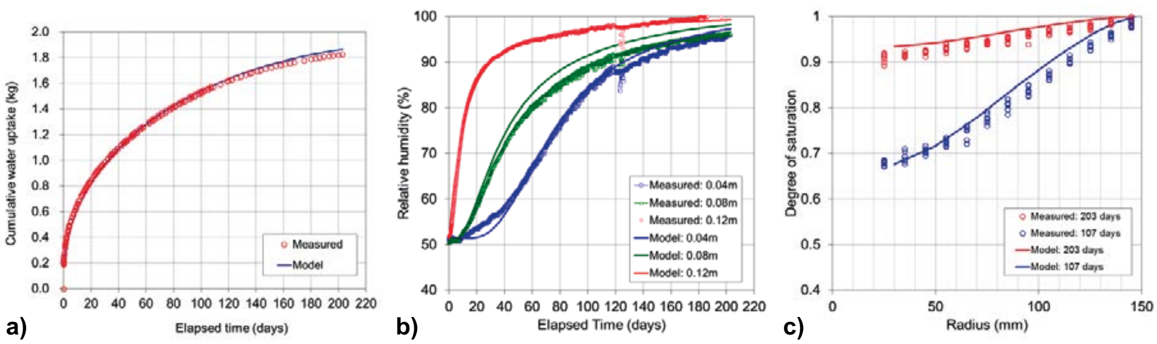


Figure 2-25. *Comparison between measured and calculated a) cumulative water-uptake, b) relative humidity, and c) saturation (from Sawada et al. 2019).*

2.3 Modelling group: KAERI

2.3.1 Introduction

The Task 8A–D modelling work performed by the Korea Atomic Energy Research Institute (KAERI), Korea, is documented in Kim et al. (2018).

2.3.2 General modelling approach

KAERI used a conventional continuum approach to simulate both the fractured rock and partially saturated bentonite in a single run. Analytical solutions were used as part of the Task 8A verification study.

2.3.3 Task 8A

A radially symmetric model was developed to represent the deposition hole and surrounding formation. Geometry and material properties were taken from the task description (Vidstrand et al. 2017). The results were compared to those obtained by Code_Bright as reported in Vidstrand et al. (2017) and the analytical solution by Börgesson (1985), which assumes (unlike the numerical solutions) a constant hydraulic diffusivity; the comparison is shown in Figure 2-26. The impact of a single horizontal fracture on bentonite wetting was also examined, with focus on the saturation profile at the interface between the rock and the bentonite (Figure 2-27). The effects of a rock fracture on the re-wetting of bentonite with an initially high capillary suction were appropriately represented by the TOUGH2 code.

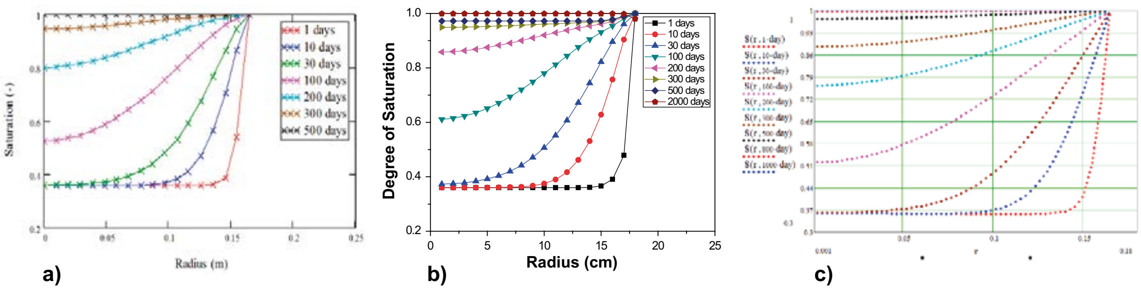


Figure 2-26. Radial saturation distribution calculated by a) Code_Bright (Vidstrand et al. 2017), b) TOUGH2, and c) the analytical solution (Börgesson 1985) (from Kim et al. 2018).

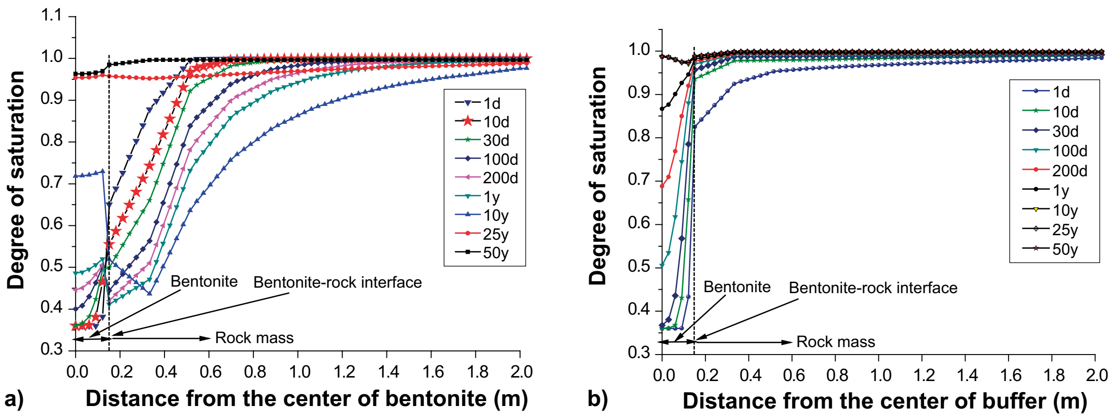


Figure 2-27. Radial distribution of saturation around the bentonite-rock interface a) without and b) with a horizontal fracture (from Kim et al. 2018).

2.3.4 Task 8B

KAERI examined multiple approaches to the problem of simulating water flow in a formation that contained large discrete geologic structures described deterministically, smaller fractures that need to be described stochastically, or a combination thereof (Figure 2-28). A FracMan/MAFIC model was developed for each of these cases to calculate saturated water inflow into a tunnel. From this flux, an equivalent permeability was determined and assigned to a homogeneous TOUGH2 model used for simulating bentonite re-saturation. Inflow to open boreholes was simulated with each conceptualization. With the given assumptions on the transmissivity of the large and individual small fractures, the results indicated that most of the inflow occurs through the stochastic fracture network. Bentonite re-saturation was calculated for a simplified configuration with a single deterministic fracture interesting the borehole.

2.3.5 Task 8C

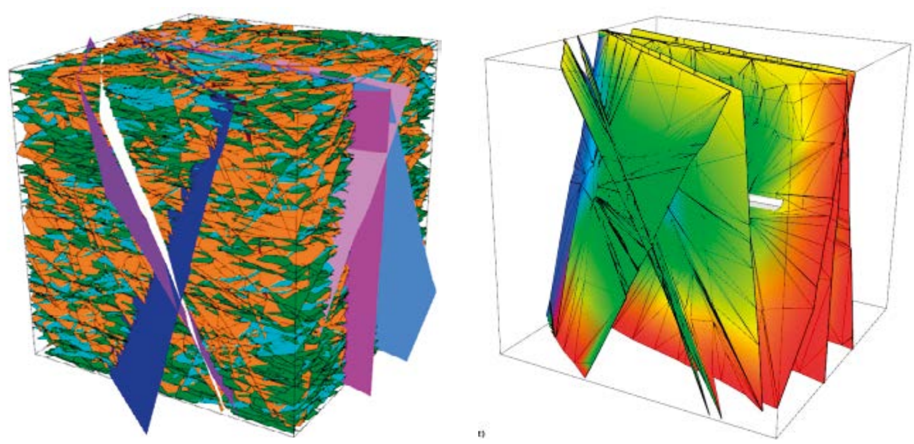
A complex series of model runs (using different codes) was used to arrive at an effective permeability to be used for the ultimate simulations. A DFN was generated and then mapped onto a FLAC3D grid, whereby element-specific effective permeabilities were calculated using a volume-averaging technique referred to as the "smeared fracture model". Steady-state inflow into the probing holes and the 300-mm diameter surrogate deposition holes (Task 8C1) was performed for the conceptualizations described in Section 2.3.4. Bentonite re-saturation was simulated using TOUGH2 based on a homogeneous, equivalent continuum model.

It was concluded that the far field can be represented by an equivalent continuum, and that large discrete structures should be implemented deterministically. Given uncertainties in the assumption about the transmissivities of individual fractures used in the DFN to calculate effective permeabilities in the proposed multi-step approach, it is still necessary to perform a calibration step against field data to determine the effective continuum permeability.

2.3.6 Task 8D

The approach of Task 8C was used for Task 8D with a more detailed mesh geometry (Figure 2-30) and updated reference parameters. The results showed a substantial decrease in inflow compared to the simulations of Task 8C, which was attributed to a changed pressure distribution caused by additional observation holes included in the revised model. These monitoring boreholes were (mistakenly) assumed to be open; the results were therefore not considered valid.

It was concluded that the details of water-conducting features (boreholes and large fractures) on the pressure distribution is significant and needs to be taken into account for an accurate simulation of deposition hole inflow and bentonite re-saturation. A calibration step using field data is considered necessary.



a) b)

Figure 2-28. Deterministic and stochastic fractures; b) pressure distribution in deterministic, large fractures (from Kim et al. 2018).

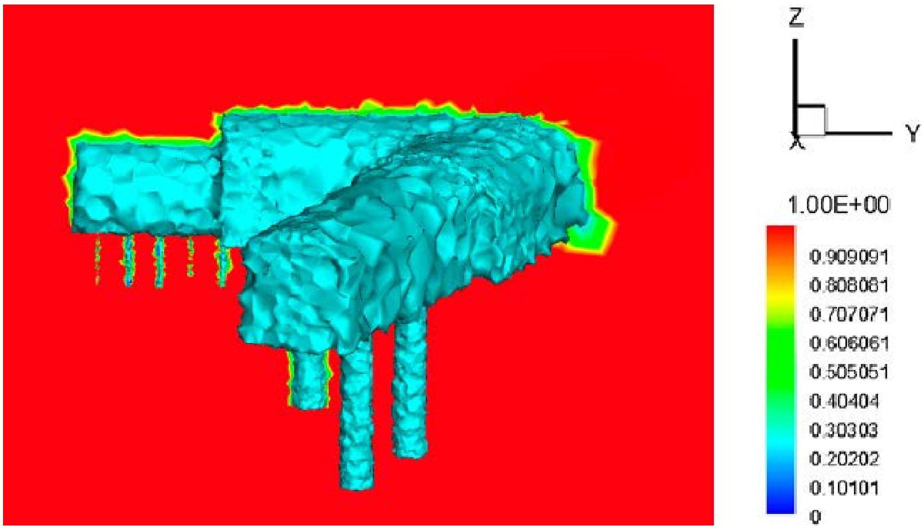


Figure 2-29. *Saturation distribution around TASO tunnel (from Kim et al. 2018).*

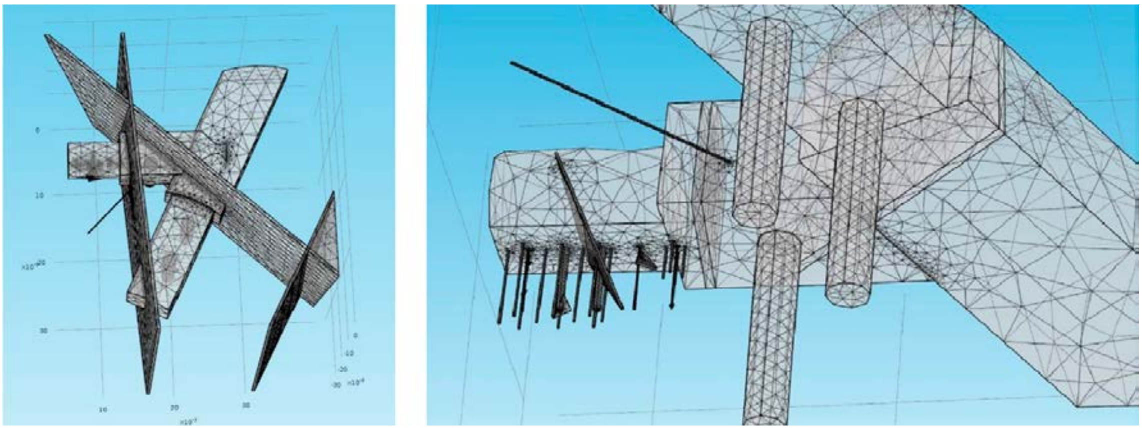


Figure 2-30. *Model geometry used for Task 8d (from Kim et al. 2018).*

2.3.7 Concluding remarks

The proposed modelling approach was able to properly describe the inflow variation into deposition holes and the re-wetting process of bentonite in fractured rocks. The inflow and bentonite re-saturation were highly influenced by the localized water inflow through fractures intersecting surrogate deposition holes. Thus it is important to identify the site-specific geological structure around the deposition hole and appropriately evaluate the impact of rock fractures. Due to the heterogeneity and complexity of the natural system, the developed model should be adjusted and calibrated with laboratory and field data for better prediction and increased reliability.

KAERI is currently involved in complementary studies at the In-DEBS (In-situ Demonstration of Engineered Barrier System) experiment at the KURT facility in Korea.

2.4 Modelling group: LANL

2.4.1 Introduction

The modelling work performed by Los Alamos National Laboratory (LANL), United States, is documented in Dittrich et al. (2014). LANL only addressed the mesh generation aspect of Task 8D.

2.4.2 General modelling approach

LANL developed and explored a discretization technique that allows connecting a discrete fracture network model (DFN) consisting of 2D fracture volume elements to 3D elements representing the bentonite in the deposition hole. The DFN model contained fractures only. Fractures were meshed by a 2D polygonal control volume grid in a 3D simulation domain. The background rock between fractures was not considered. However, modelled bentonite boreholes were represented as cylindrical 3D objects and meshed by 3D tetrahedrons. The computational meshes were referred to as a hybrid DFN/volume grids to simulate fluid flow coming from 2D fractures into 3D bentonite boreholes. Figure 2-31 shows the step-by-step methodology used for hybrid mesh generation. Unsaturated and two-phase flow within the hybrid DFN/volume grids was calculated using the FEHM simulator.

2.4.3 Task 8D

The primary goal of the work was to gain experience in applying the hybrid DFN/volume gridding approach to a realistic, complex configuration. Two realizations of a DFN were generated based on fracture statistics given in the task description (Vidstrand et al. 2017), including three deterministic fractures. Tunnels were represented by atmospheric boundary conditions; bentonite-filled deposition holes were represented by 3D tetrahedral volume elements.

Initial results for rewetting of the bentonite for two realizations of the DFN are shown in Figure 2-32. Both realizations show a steep gradient in liquid saturation in the bentonite near where it intersects with fractures. Away from that intersection, the bentonite is rewetting relatively uniformly.

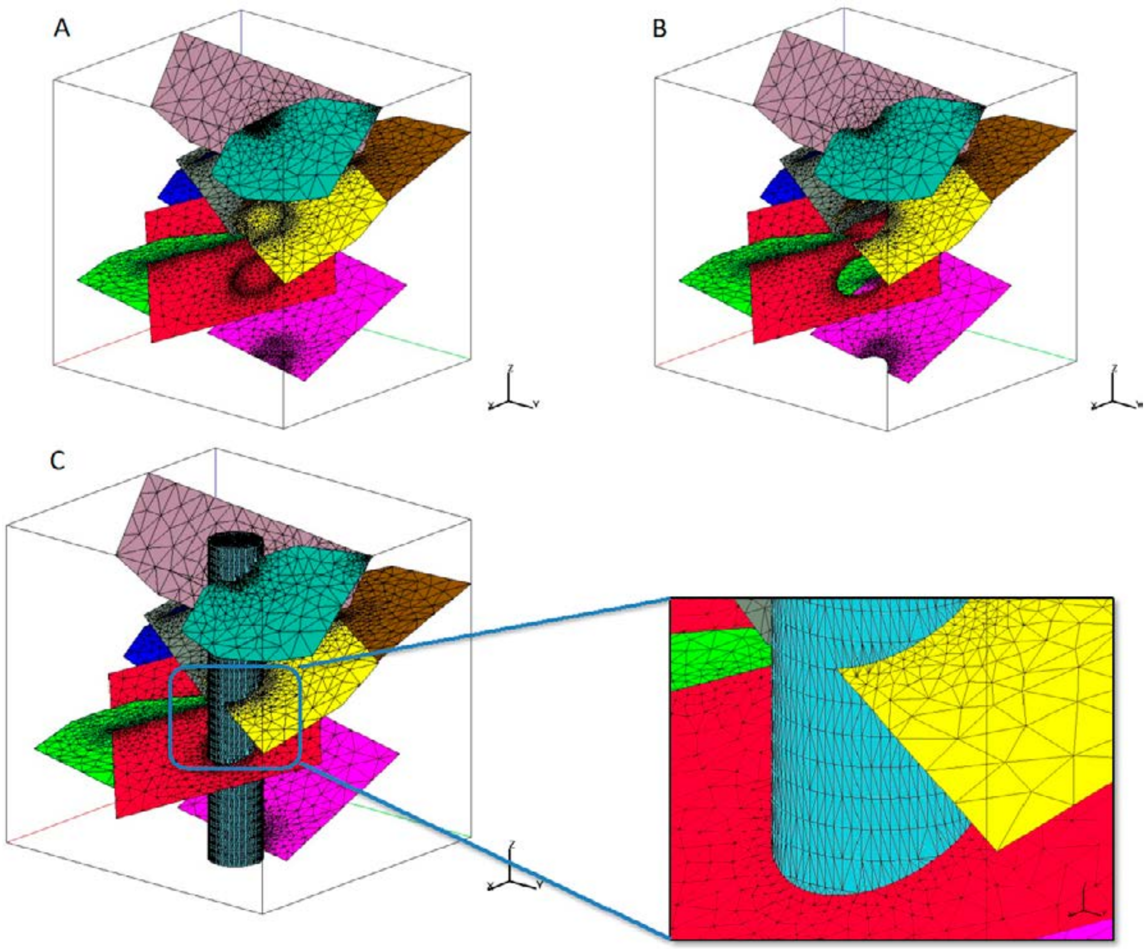


Figure 2-31. *Example showing the creation of a hybrid tetrahedral/DFN mesh (from Dittrich et al. 2014).*

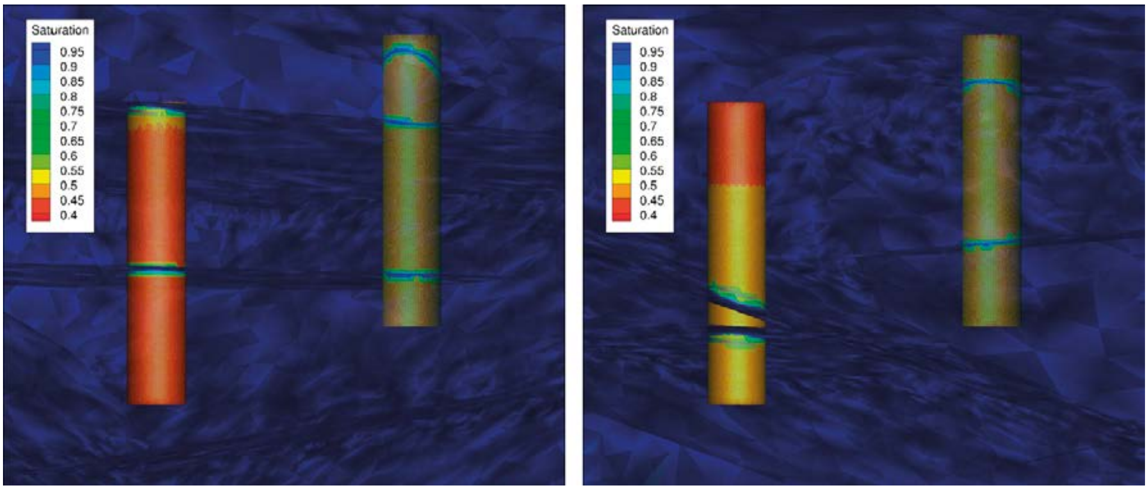


Figure 2-32. *Saturation distribution after 3 months, simulated with hybrid DFN/Volume grid approach for two DFN realizations (from Dittrich et al. 2014).*

2.4.4 Concluding remarks

The DFN with boreholes in place demonstrates a modelling capability that combines volumes and DFN meshes for the incorporation of complex geometries. Little difference was noted between the overall behaviour of the two DFN realizations.

2.5 Modelling group: NDA-AMEC

2.5.1 Introduction

The Task 8C modelling work performed by AMEC, United Kingdom, is documented in Baxter et al. (2014a, 2018a); the Task 8D modelling work is documented in Baxter et al. (2014b, 2018b).

2.5.2 General modelling approach

AMEC combined saturated discrete fracture network (DFN) modelling with two-phase continuum modelling to simulate re-saturation of bentonite emplaced in fractured rock. Given that DFN models are constrained by the resolution of field data used for parameterisation (e.g. small fractures intersecting a tunnel may not be mapped), and that the background matrix (including fractures neglected in the DFN) may be relevant for bentonite wetting in deposition holes with limited fracture intersections, an effective continuum approach based on the TOUGH2 code was also examined to simulate bentonite wetting. In this second approach, the ConnectFlow DFN code was used to determine porosities and permeability tensors, which were then mapped onto the TOUGH2 continuum grid.

2.5.3 Task 8C

The conceptual models for Tasks 8C1 and 8C2 were quite different. For Task 8C1, which is concerned with inflow into open probing holes, the DFN model was directly used to calculate single-phase fresh-water flow through the fractured bedrock. Three significant fractures were included deterministically. The DFN was not conditioned or calibrated. All mapped fractures were considered hydraulically active. Ten realizations of the DFN were simulated. Inflows to open boreholes were also calculated using the heterogeneous TOUGH2 model.

For Task 8C2, two-phase flow of saline groundwater was simulated using TOUGH2, with equivalent element-by-element kinematic porosities and directional permeabilities (Figure 2-33) estimated by calculating the flux through the DFN for a linear head gradient in each of the axial directions. Diffusion of water vapour, brine, and air was also accounted for. In addition to the heterogeneous continuum model using the upscaled DFN properties, simulations were performed for a homogeneous case with permeability set as the geometric mean of the upscaled permeabilities, and for different background rock permeability values.

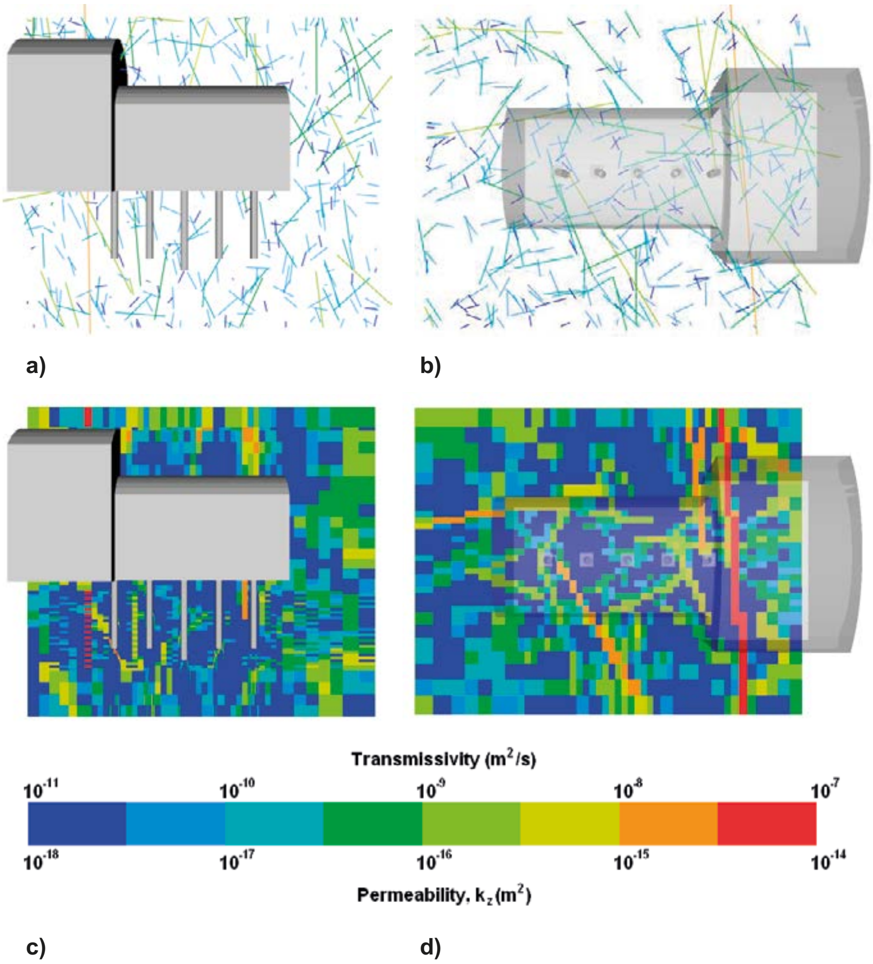


Figure 2-33. *Transmissivity (m^2/s) (a,b) and upscaled permeability (m^2) (c,d) in the deposition hole near-field. For (a,c) a vertical slice through all five probing boreholes is represented; and for (b,d) a horizontal slice is taken at an elevation of −418 m. Results are shown for the second realisation of the stochastic fracture network (from Baxter et al. 2014a, 2018a).*

Inflow to five boreholes, which were individually or collectively open, was simulated for 10 DFN realizations. While the average inflow from the 10 realizations considerably overestimated inflows to each borehole (see Figure 2-34), Realization 2 was in reasonable agreement with the measured data and was thus selected for more detailed analyses (see Figure 2-35).

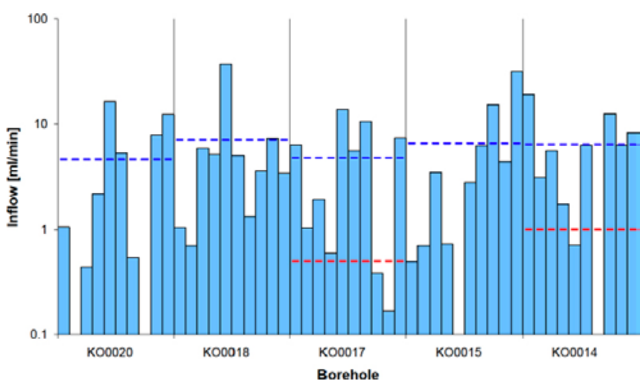


Figure 2-34. *Inflows for each of the 10 flow simulations, where each borehole is opened in turn. The average inflow is shown in dark blue, and observed groundwater inflow is shown in red (from Baxter et al. 2014a, 2018a).*

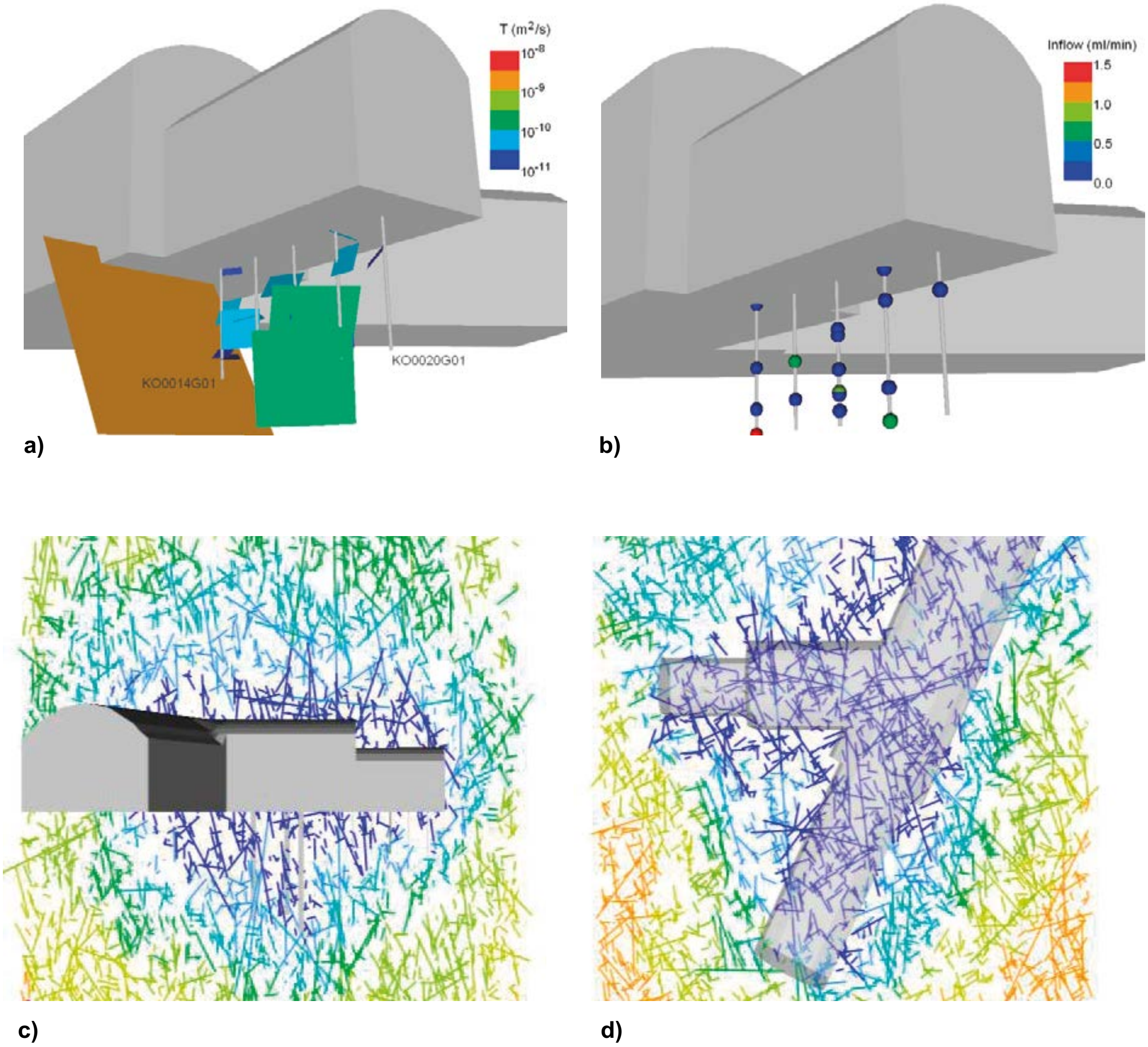


Figure 2-35. *Realisation 2 of the stochastic fracture network, illustrating a) the local fracture tessellates coloured by transmissivity, b) inflow points, as well as near-field pressure distributions for c) a vertical slice through all five boreholes, and d) a horizontal slice at an elevation of −418 m (from Baxter et al. 2014a, 2018a).*

Inflow into open and bentonite-filled surrogate deposition holes was calculated using the heterogeneous TOUGH2 model. Pressure and saturation distributions after 1 year are shown in Figure 2-36.

Comparison between the homogeneous and heterogeneous simulations (the latter based on upscaled effective parameters derived from a DFN) indicated that heterogeneity leads to potentially significantly longer bentonite wetting times, with considerable variability between boreholes and between different realizations of the underlying DFN. Capturing heterogeneity is thus considered essential, with the location of inflow points being equally important as the inflow rate. The permeability of the rock mass in between the discrete fractures is also considered influential on the estimated re-saturation time.

The proposed approach that involves DFN simulations for generating upscaled continuum properties was considered appropriate to simulate the re-saturation of bentonite emplaced in sparsely fractured bedrock.

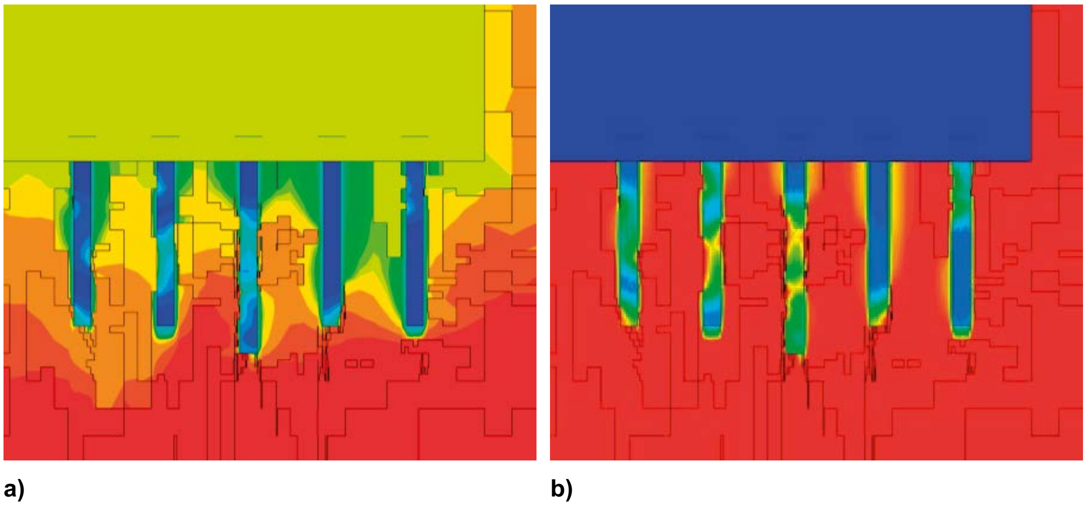


Figure 2-36. *a) Pressure and b) saturation distributions after 1 year of re-saturation for DFN Realisation 2 for a vertical slice including the deposition holes (from Baxter et al. 2014a, 2018a).*

2.5.4 Task 8D

The main difference between the model setup for Tasks 8C and 8D is the refinement of the deterministic structures, and the conditioning of the DFN to facture traces and intersection counts observed in the adjacent tunnels and deposition holes, respectively. Moreover, observed water-conducting fractures intersecting the surrogate deposition holes were deterministically included in the model. Hydraulic test data were available for model calibration. Multiple variants of the base-case model were developed to examine the impact of uncertainties in fracture intensity, fracture size-transmissivity correlation, geometry of one of the large deterministic structures, and fractures intersecting the deposition holes. Specific storage and initial bentonite saturation were updated; bedrock parameters were changed based on newly available data.

The stochastic DFN was calibrated against observed trace counts and inflows by adjusting the fracture intensity and fracture size-transmissivity distribution (Figure 2-37). Moreover, the geometry of one of the large deterministic fractures as well as smaller fractures intersecting the deposition holes were adjusted to match inflow and pressure build-up data.

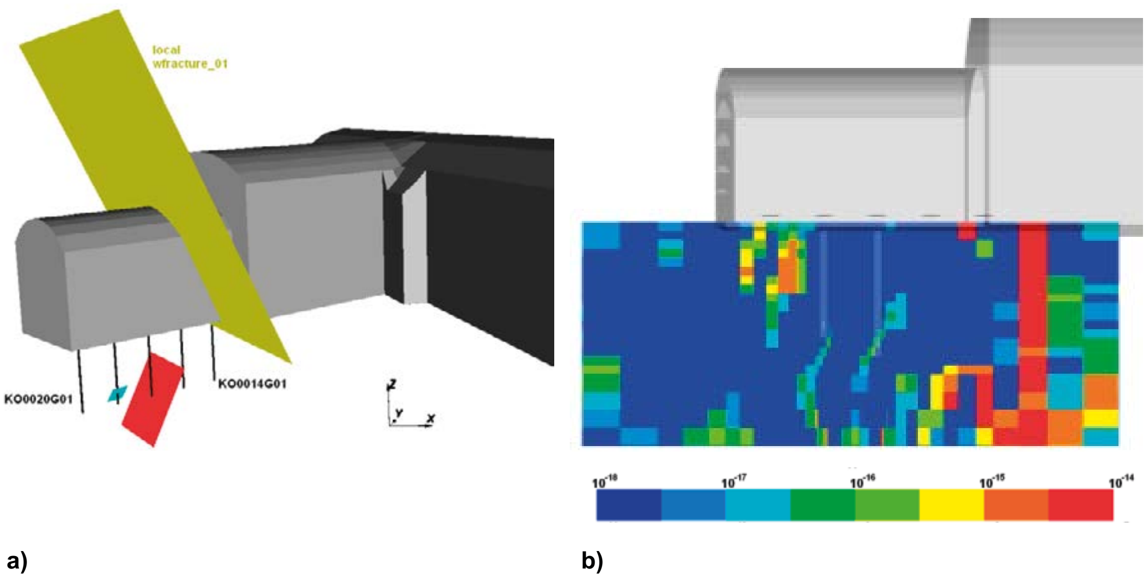


Figure 2-37. *a) Deterministically specified fractures used to represent the identified inflow locations in overcored boreholes, and b) upscaled permeability (m^2) in the deposition hole near-field (from Baxter et al. 2014b, 2018b).*

The variant most closely reproducing observed data was used for predicting flow through the rock (represented as a heterogeneous equivalent porous medium), inflow into open deposition holes, and re-saturation of emplaced bentonite (Figure 2-38).

The evolution of pressures and saturations in the bentonite and surrounding fractured rock were examined for various realisations, variants, and parameter perturbations. Results were compared to measured relative humidity data, showing the impact of assumptions about rock and bentonite permeabilities. Model results were summarized by providing ranges of predicted inflows and re-saturation times. Conceptual assumptions were discussed in the light of qualitative comparisons to experimental data.

2.5.5 Task 8F

For Task 8F, the previously developed model was further refined by a) removing stochastic fractures near the boreholes, b) instead deterministically specifying the water-conducting fractures intersecting the reamed surrogate deposition holes, and c) conditioning the model to the responses of the relative humidity sensors. Unlike in Tasks 8C and D, the simulations were performed using ConnectFlow based on Richards' equation rather than the two-phase formulation of TOUGH2. For Subtask 8F1, the fractured bedrock was represented explicitly, and steady-state, saturated flow was calculated to the open surrogate deposition holes. One hundred realisations of the stochastic DFN were examined. The calculated inflows to boreholes were compared to measured data (see Figure 2-39) to select the networks used for simulating bentonite wetting.

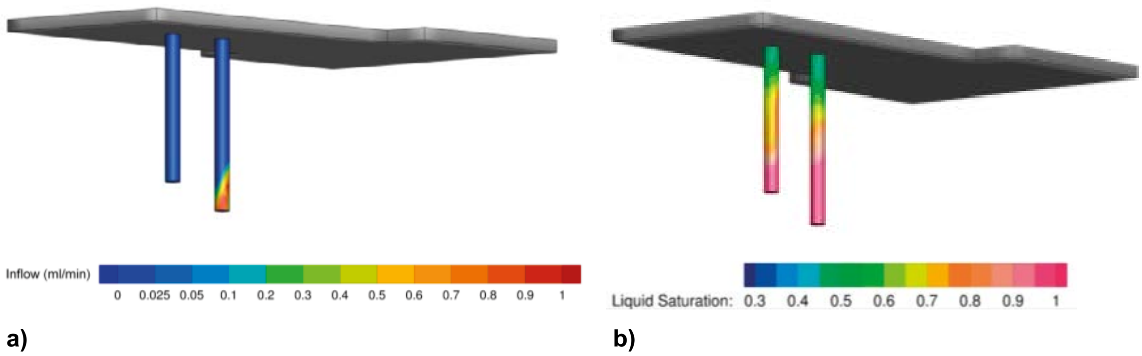


Figure 2-38. *Examples of simulated a) steady-state inflow into open deposition holes, and b) saturation at bentonite surface after 1 year of rewetting (from Baxter et al. 2014b, 2018b).*

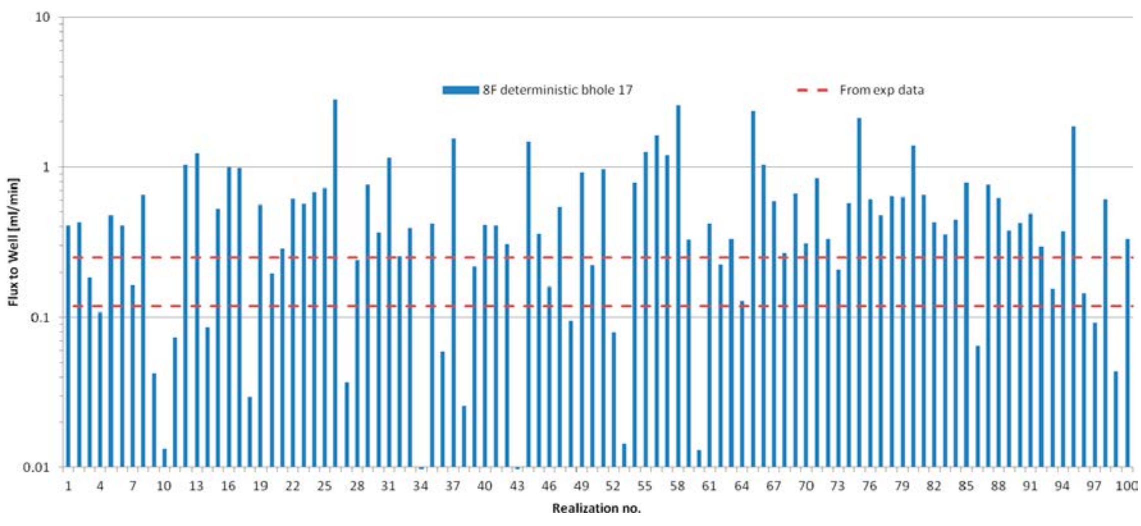


Figure 2-39. *Inflow in KO0017G01 evaluated for 100 different realizations of the fracture network. The red dashed lines limit the experimental band of values found during the experimental phase (from Baxter et al. 2016, 2018c).*

For Subtask 8F2, the transient re-saturation of bentonite was simulated using the continuum approach. Bentonite properties were determined based on relative humidity data. The conditioned model was then used for the prediction of bentonite re-saturation up to the time of excavating the BRIE, at which point the model results were compared to the corresponding water-content measurements (see Figure 2-40).

Sensitivity analyses examined the effects of relative permeability and hydraulic diffusivity on bentonite wetting to estimate these parameters in the dry region of the bentonite, i.e. in the absence of fractures. Finally, the long-term evolution within the bentonite and the surrounding bedrock was examined.

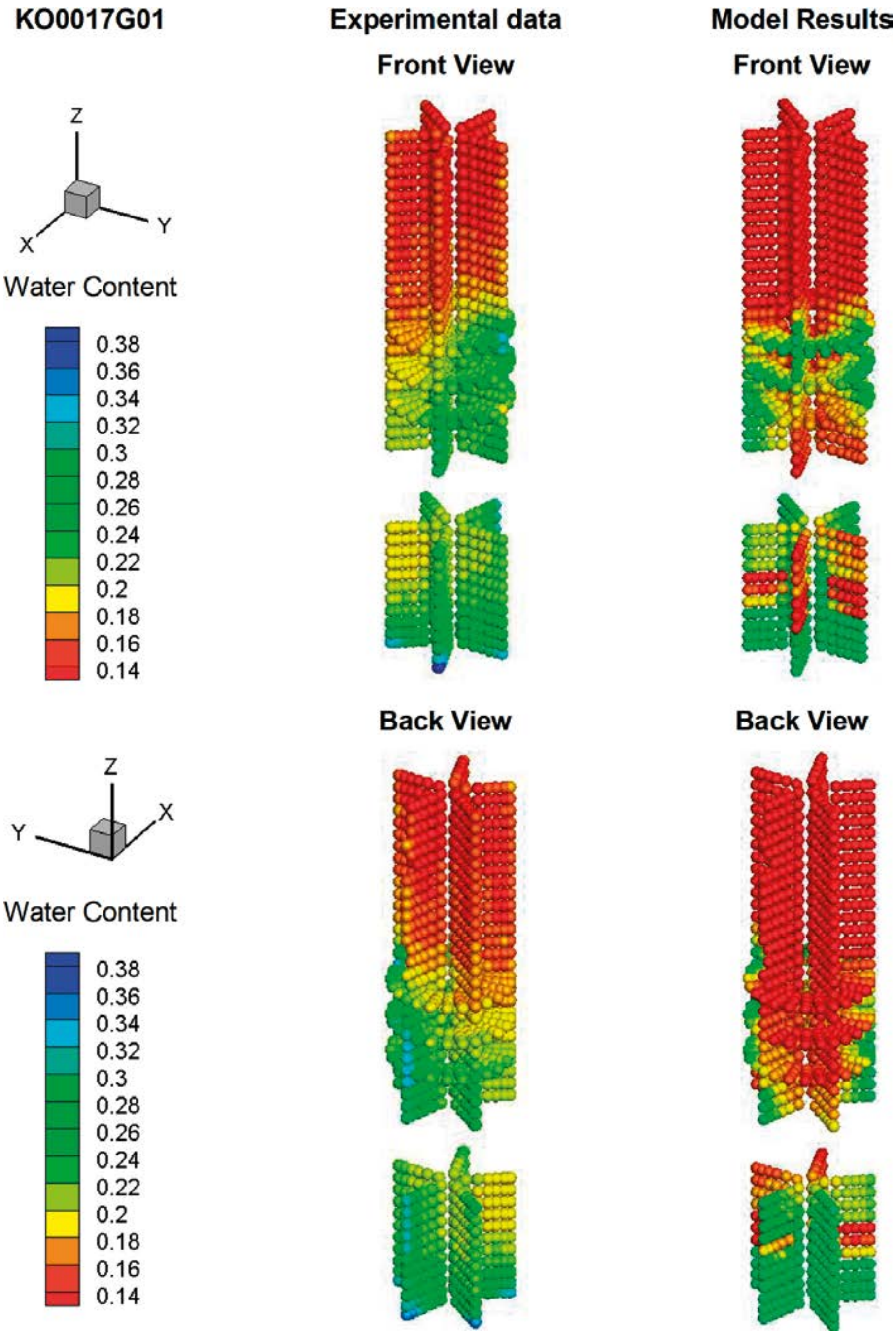


Figure 2-40. *Scatter plot of water content in borehole KO0017G01 from experimental data and model results (from Baxter et al. 2016, 2018c).*

2.5.6 Concluding remarks

AMEC reached the following main conclusions:

- A methodology was developed for conditioning models of bentonite emplaced in heterogeneous, fractured bedrock.
- Detailed characterisation of geometric and hydraulic properties of the fracture network is essential, specifically in the near field, allowing for a conditioning of the network to the fractures intersecting the deposition holes.
- The permeability of the background rock is also significant to understanding the re-saturation times and profiles of emplaced bentonite, with predictions very sensitive to changes in the background rock parameterisation.
- Calibrating and conditioning the underlying fracture network can substantially reduce uncertainty in the re-saturation rates and profiles of the bentonite, and improve the comparison between model results and experimental wetting data. However, the parameterisation resulting from model conditioning is inherently non-unique.
- Both bentonite and background rock permeabilities significantly influence re-saturation times.
- The physical properties of the bentonite are important parameters in the prediction of the re-saturation times of the emplaced bentonite.
- BRIE provided a comprehensive data set for understanding and refining generic methodologies developed to represent the interaction between the groundwater flow from the rock and the re-saturation of the bentonite.
- It may be advantageous to include heterogeneity in the background rock, along with a very detailed description of inflow characteristics into the deposition holes using a micro-structural model.

2.6 Modelling group: Posiva-VTT

2.6.1 Introduction

The Task 8 modelling work performed by Posiva-VTT, Finland, is documented in Pulkkanen (2018).

2.6.2 General modelling approach

Both the natural and engineered barrier systems were simulated using a single model based on the same approach to calculate (potentially unsaturated) flow in the geosphere and bentonite re-saturation. The two subsystems were thus fully coupled. The bedrock including its fractures as well as the bentonite were considered to be porous materials with effective or equivalent continuum properties.

2.6.3 Task 8A

Posiva-VTT used Task 8A as a model-development and testing exercise, in which the performance of two simulators, COMSOL Multiphysics and TOUGH2 (Pruess et al. 1999) was examined. The saturation distributions and bentonite wetting times calculated by the two simulators were considered consistent with each other, even though they differed slightly, which was attributed to the use of different relative permeability functions and quite different grid resolutions. Moreover, the numerical schemes to handle phase transitions (from fully saturated to partially saturated conditions) were different between the two codes.

The flexibility offered by COMSOL to represent complex geometries, and the ease with which governing equations can be adapted, were the main reasons to select COMSOL for the remaining Task 8 exercises.

2.6.4 Task 8B

An effective continuum model that incorporates both the geosphere and the surrogate deposition hole (first open, then backfilled with bentonite) was developed, whereby the large geologic structures were implemented as 10-cm thick planar bodies with permeabilities that were higher than that of the bedrock, which was assumed to be homogeneous. Steady-state conditions established with open deposition holes were used as initial conditions for the subsequent simulation of bentonite wetting. Richards' equation for saturated/unsaturated flow was solved using COMSOL.

Figure 2-41 shows the pressure and saturation distribution within and around the deposition hole 0.5 years after bentonite instalment, demonstrating the ability of the chosen modelling approach to simulate flow and re-saturation processes in a single model that comprises both the natural and engineered barrier systems.

The impact of the fracture was relatively minor because water was also supplied through the background rock; the wetting time was predicted to be on the order of 1 year.

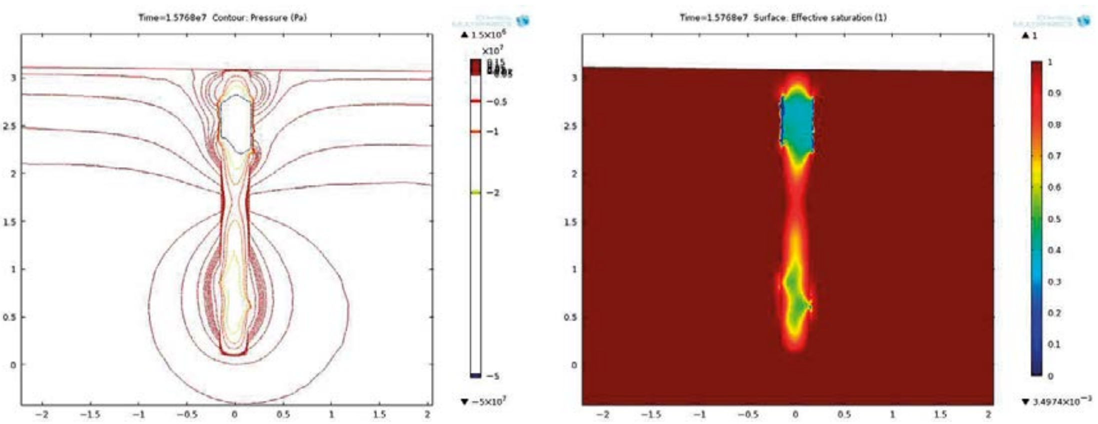
2.6.5 Task 8C

The conceptual model included 1) three large discrete geologic structures, 2) underground openings, specifically probing and surrogate deposition holes, that were 3) surrounded by a skin zone, which 4) was cut by two-dimensional, ellipsoidal fractures discretely inserted based on borehole imaging processing system (BIPS) data, and 5) a homogeneous equivalent porous medium elsewhere (Figure 2-42).

Equivalent permeabilities of the bedrock and transmissivities of the small fractures near the boreholes were estimated by calibrating the model against inflow data to the TASO tunnel and measured inflows to the open boreholes, respectively.

Bentonite re-saturation was then calculated using the calibrated model (Figure 2-43). Wetting times up to 60 years were calculated, depending on the position of the fractures intersecting the borehole, which in turn affected the properties determined by model calibration.

In addition to detailed characterisation of the geometry of inflow from the fracture network to the bentonite surface, a good understanding and reliable parameters describing the wetting behaviour of the bentonite were considered essential for making robust predictions of re-saturation times.



a) b)

Figure 2-41. Simulated a) pressure and b) saturation distribution in bentonite 0.5 years after bentonite emplacement; the fracture zone intersects the deposition hole 1.5 m below the tunnel floor (from Pulkkanen 2018).

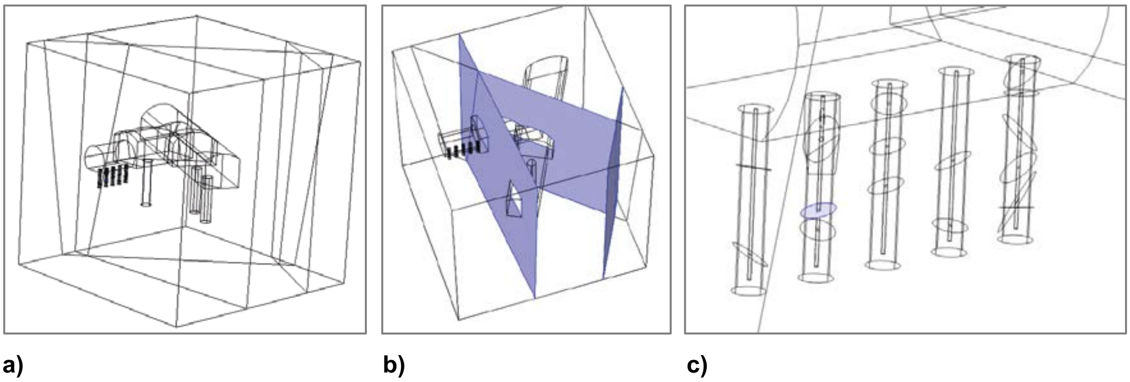


Figure 2-42. *a) Model geometry, b) discrete large structures, and c) discrete small fractures intersecting boreholes (from Pulkkanen 2018).*

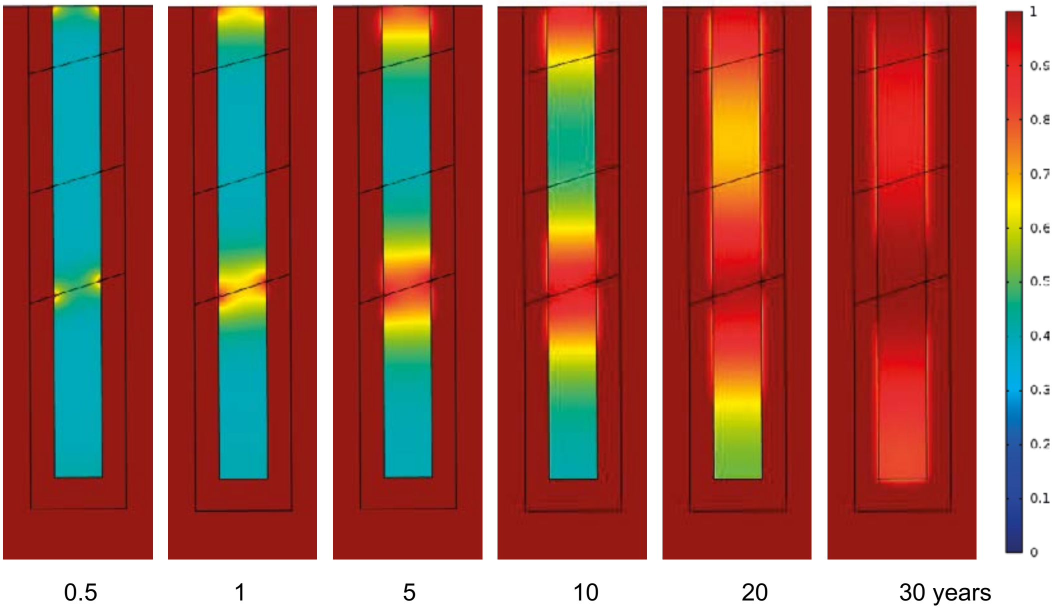
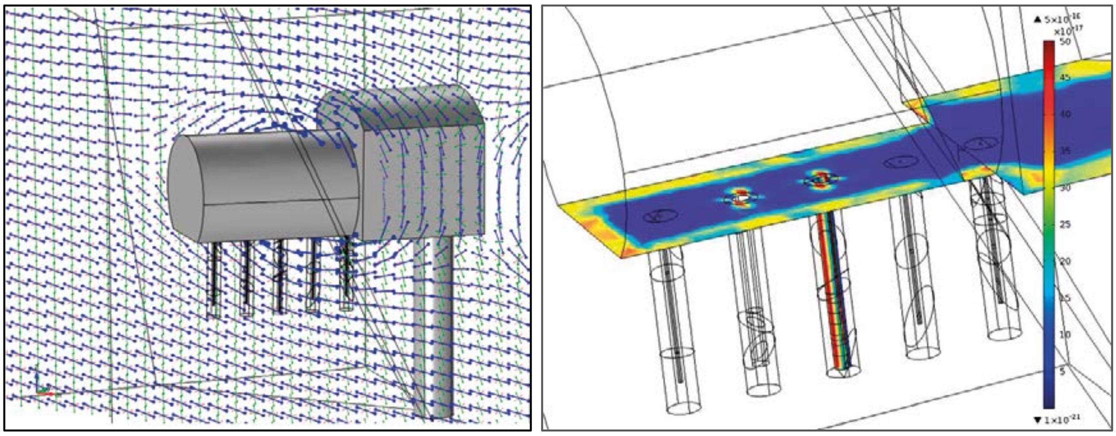


Figure 2-43. *Saturation of bentonite at different times (years) (from Pulkkanen 2018).*

2.6.6 Task 8D

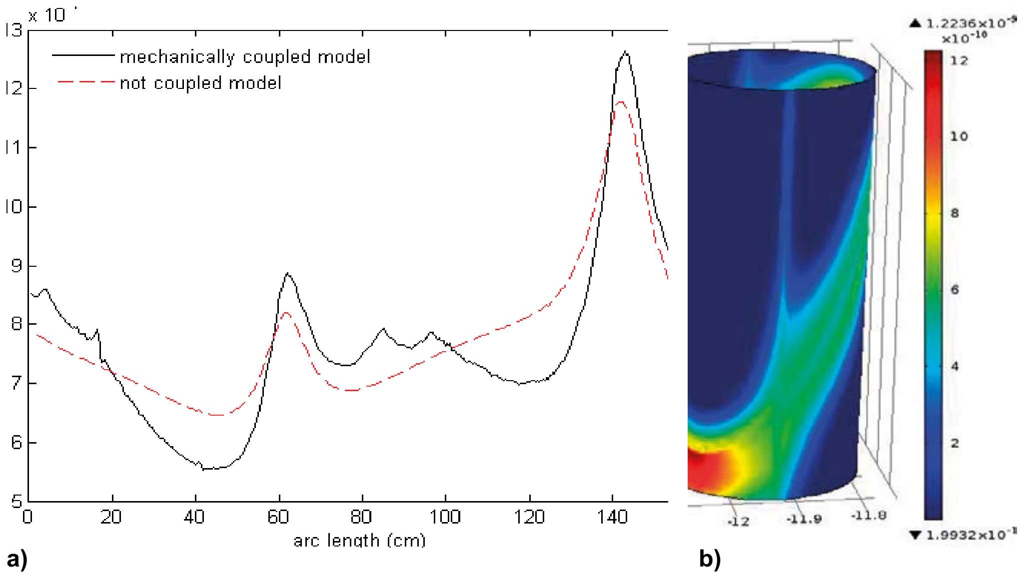
Relative to Task 8C, the model domain was reduced to a 20^3 m^3 cube. Moreover, the location of some of the deterministic fractures and the number of small fractures was updated. Mechanical processes were added to the conceptual model to examine the impact of deposition hole drilling on properties and inflow. Consequently, no *a priori* skin zone was specified, as its existence and properties were the objective of the modelling. The mechanical model was uni-directionally coupled to the flow model; different submodels for both fractures and bedrock were examined (Figure 2-44). Inflow characteristics obtained with the different mechanical models were examined and compared to measured data in an attempt to identify the most likely conceptual model.

The model was calibrated using inflow data before predictions of the bentonite re-saturation were made. Specifically, measured inflows to the TASO tunnel floor and into Borehole 17 were used to estimate bedrock and fracture permeabilities. The mechanical coupling appeared to have a minor effect on bentonite re-saturation (Figure 2-45), even though it allowed for a better reproduction of the observed inflow patterns. A wetting time on the order of 1 year was obtained, suggesting that the contribution from the bedrock (despite a reduced permeability) dominated the re-saturation process, which was also confirmed by comparison to the pattern seen in the relative humidity data.



a) b)

Figure 2-44. Impact of a) principal strain on b) permeability along principal stress direction (from Pulkkanen 2018).



a) b)

Figure 2-45. a) Inflow pattern through the fracture intersecting Borehole 17, and b) flow velocity from background rock (from Pulkkanen 2018).

2.6.7 Task 8F

Based on the insights gained from Task 8D, the conceptual model used to reproduce the wetting behaviour observed after dismantling of BRIE was slightly simplified. In particular, the location and dip of the larger fractures intersecting Boreholes 17 and 18 were adjusted, whereas the smaller water-conducting features (including the pegmatite vein), which only exerted a local effect on bentonite wetting, were discarded. As a consequence, the permeability of the background rock was very low, i.e. wetting was dominated by the main fractures. Mechanical coupling was not included, as its effect on bentonite wetting was demonstrated to be minor. The model was calibrated against inflow to the TASO tunnel, open boreholes, and relative humidity data (Figure 2-46) by updating the hydraulic conductivity of the background rock and the bentonite wetting model parameters.

2.6.8 Water-uptake test

The water-uptake test (WUT) was modelled using a cylindrical model filled with uniform bentonite at an initial suction pressure of −67 MPa and a radial boundary pressure of 0.1 MPa. Bentonite properties were identical to those used in Task 8D. Cumulative water-uptake, saturation profiles and relative humidity were well reproduced by the model (Figure 2-47.

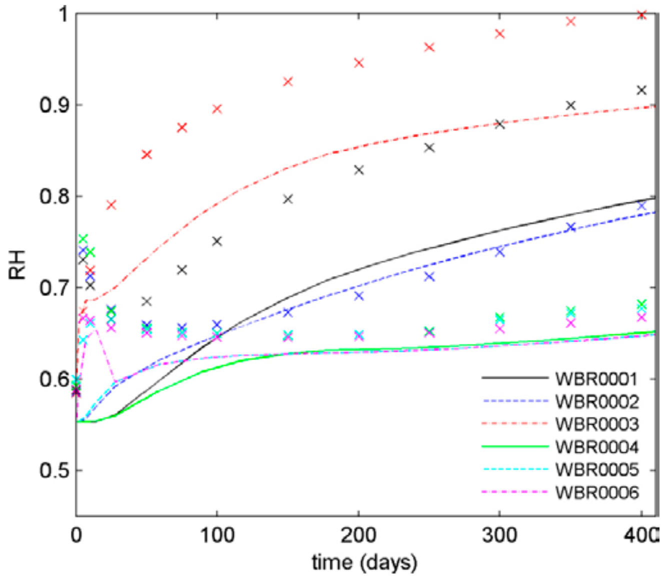


Figure 2-46. *Measured (symbols) and simulated (lines) relative humidity evolution at various sensor locations (from Pulkkanen 2018).*

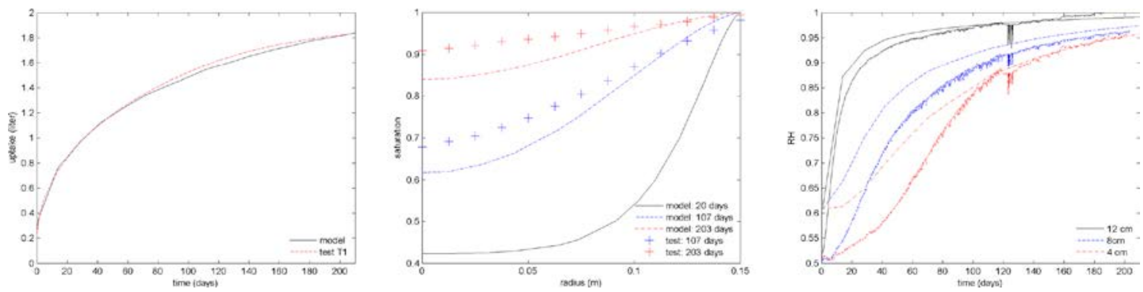


Figure 2-47. *Measured and simulated a) cumulative water-uptake, b) saturation profiles, and c) relative humidity from water-uptake tests (from Pulkkanen 2018).*

2.6.9 Concluding remarks

Posiva-VTT developed a hybrid modelling concept that combined discrete fractures and features at the bentonite rock interface and an equivalent porous medium (EPM) approach in the far field to represent the connected fracture network. The key components of the model were the bentonite filled borehole, the small discrete fractures and pegmatite vein cutting the boreholes, the low permeable zone around the boreholes, the large deterministic fractures, and the connected fractured bedrock where the EPM concept was used. Based on the comparison between the calculated and observed bentonite wetting rates, it was concluded that the pegmatite vein should be removed, and that the hydraulic conductivity of the rock mass was likely on the order of that of intact rock matrix. As a result, the effect of the small fractures could not be averaged to form an equivalent porous medium around the borehole; they had to be included explicitly. The longest dry section between water-supplying fractures thus determined bentonite wetting. The relative permeability and capillary pressure functions used for bentonite need to be re-evaluated as they produce strong gradients at the rock-bentonite interface that were not observed after dismantling of BRIE. The mechanical coupling of the bedrock hydraulic model proved to be useful mostly when examining the inflow to open boreholes. However, the relatively small deviations in the hydraulic parameters for bedrock resulting from hydromechanical effects had a limited effect on bentonite wetting, which was dominated by bentonite properties.

2.7 Modelling group: SKB-CFE-Golder

2.7.1 Introduction

The Tasks 8A, 8C, and 8D modelling work performed by Golder Associates AB, Sweden, and Computer-Aided Fluid Engineering AB, Sweden, is documented here.

2.7.2 General modelling approach

The modelling was performed with the code DarcyTools (Svensson et al. 2011), which is based on a finite volume formulation using staggered computational grids. Discrete fractures were implemented by averaging properties according to the volume fractions of a material within a grid block. Five realisations of stochastic fracture networks were generated. Unsaturated flow was implemented by adjusting specific storage.

The fractured bedrock and bentonite buffer were both simulated using the same concept within a single model, allowing for an integrated treatment of the natural and engineered barrier systems including feedback mechanisms. However, partially saturated conditions were initially only considered in the bentonite.

2.7.3 Task 8A

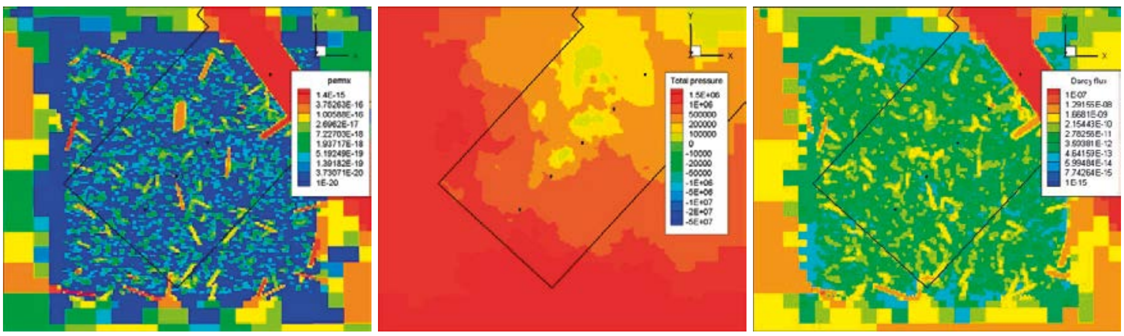
The modelling of the two cases demonstrated the capability of the modified DarcyTools simulator to handle bedrock, fractures, and bentonite in a single model, and to address unsaturated flow. The results indicated that partially saturated conditions might also develop in the fractured rock (i.e. not just the bentonite), a process that was ignored in this simulation study.

2.7.4 Task 8C

A model was developed that deterministically included the underground openings (tunnels, two surrogate deposition holes, and five probing holes) and the three large discrete features (with corrected location and extent). Discrete fractures were generated using a fracture density that was reduced by a factor of five to account for the fact that not all fractures are hydraulically active.

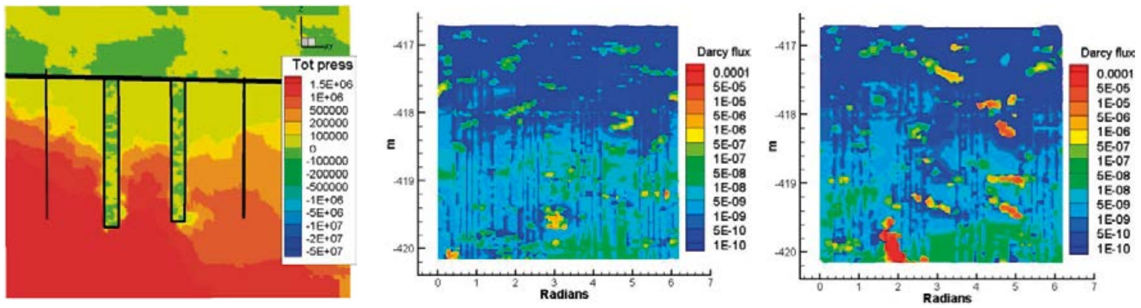
The model consisted of two domains, where the region near the boreholes exhibited a higher grid resolution. Moreover, in addition to three sets of intermediate-sized stochastic fractures, three sets of smaller fractures were generated within that near-field region.

Steady-state simulations with closed boreholes (Figure 2-48) provided the initial conditions for subsequent simulations of flow into open boreholes (Figure 2-49). Bentonite re-saturation is visualized in Figure 2-50; wetting time is on the order of one year.



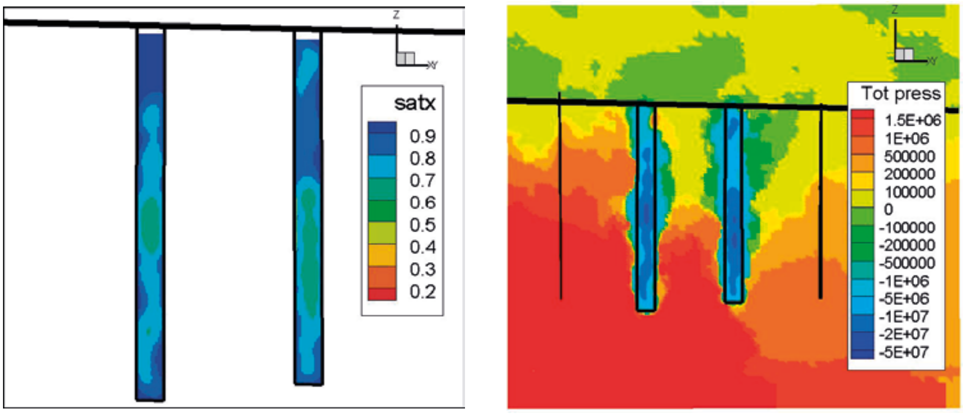
a) b) c)

Figure 2-48. *a) Permeability structure, b) pressure distribution, and c) Darcy fluxes along a horizontal section with all boreholes closed.*



a) b) c)

Figure 2-49. a) Pressure distribution of a vertical section with Boreholes KO0017G01 and KO0018G01 open, and foldup of inflow to b) borehole KO0017G01 and c) borehole KO0018G01.



a) b)

Figure 2-50. Distribution of a) saturation and b) pressure 1 year after bentonite installation.

Inflow occurred through the small fractures, i.e. fractures were more relevant than the background rock. Fracture density was thus a controlling factor, unless the borehole was intersected by one of the key deterministic geologic structures. Re-saturation times for the bentonite were also calculated. Multiple discrete fracture network realisations were simulated; the resulting standard deviations in the calculated inflow were generally larger than the mean inflow value. The random placement of fractures therefore seemed to have a large impact on the resulting inflows to the boreholes.

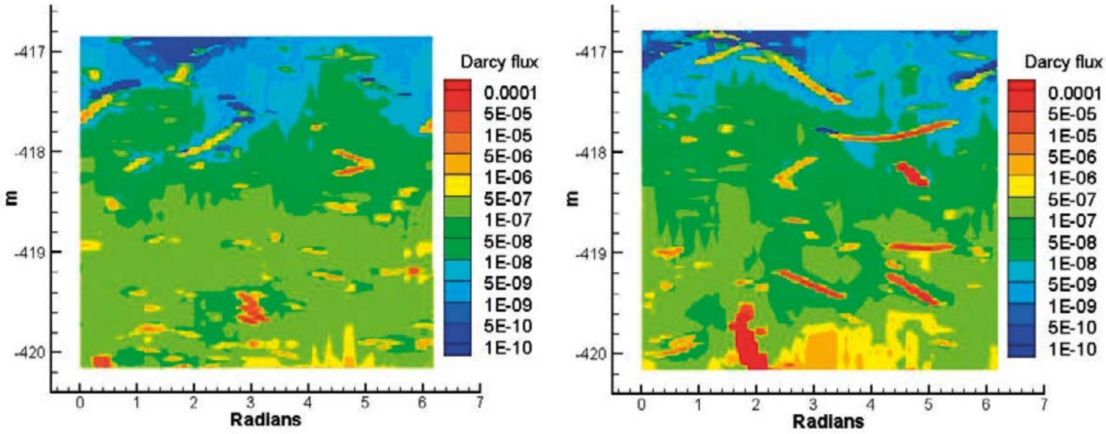
The model assumed that the bedrock was always fully saturated, which potentially misrepresented the flow across the interface between the rock and the bentonite. Potential modelling artefacts related to temporal discretisation were mentioned.

2.7.5 Task 8D

The conceptual model used for Task 8D was consistent with that for Task 8C, with the notable exception that the development of partially saturated conditions in the background rock was accounted for. Moreover, the thickness of the large discrete geologic structure was reduced from 1 m to 0.1 m, with some of the rock properties adjusted per the task description. The model was not calibrated; five realizations of the stochastic fracture network were examined.

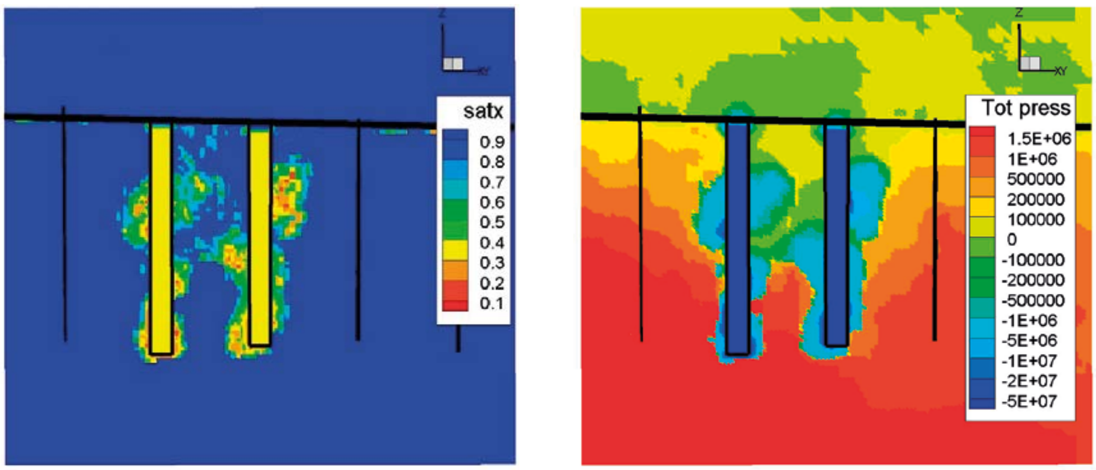
The resulting inflow distributions into surrogate deposition holes are shown in Figure 2-51, indicating localized high influxes on distinct fracture segments. Figure 2-52 shows the saturation and pressure distributions 0.1 years after bentonite installation, indicating that the rock around the deposition holes is partially saturated.

The water-uptake test was also simulated based on the simplified saturation (SIMSAT) method implemented in DarcyTools. The cumulative water-uptake was very well matched; Figure 2-53 shows a comparison between measured and modelled saturations and relative humidity.



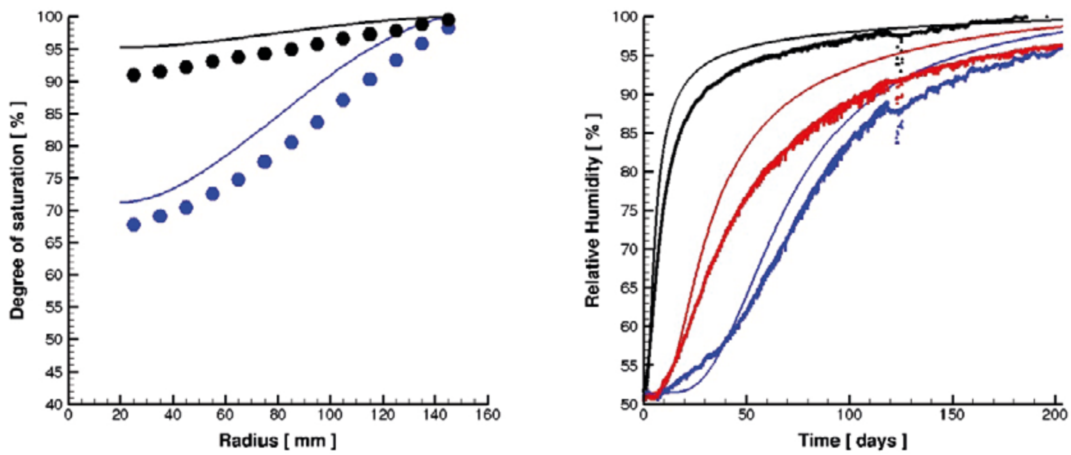
a) b)

Figure 2-51. *Foldup of inflow to a) borehole KO0017G01 and b) borehole KO0018G01.*



a) b)

Figure 2-52. *Distribution of a) saturation and b) pressure 0.1 year after bentonite installation.*



a) b)

Figure 2-53. *Comparison between modelled (lines) and measured (symbols) a) saturation profiles at two times, and b) relative humidity transients at three locations.*

2.7.6 Concluding remarks

The following conclusions were drawn:

- Inflow to open boreholes and wetting of bentonite varies considerably between realisations, indicating the influence of the stochastic fracture network.
- Large discrete geologic structures and individual fractures control the bentonite wetting process, requiring careful inclusion of site-specific data into the numerical model.
- The simulated inflows into open boreholes are on the same order as the measured data.
- Temporal discretisation significantly affects simulation results.
- The SIMSAT approach is appropriate for simulating bentonite re-saturation.

2.8 Modelling group: SKB-Clay Technology

2.8.1 Introduction

The Task 8 modelling work performed by Clay Technology AB is documented in Malmberg and Åkesson (2018). The modelling team focussed on Tasks 8A, C, D, F, and the BRIE water-uptake test (WUT). Since they performed the WUT, Clay Technology had access to additional information and insights regarding this test.

2.8.2 General modelling approach

A two-phase flow formulation as implemented in the finite element program Code_Bright was used; however, the gas pressure was fixed at 1 bar. The bedrock was conceptualised as homogeneous on the large scale and heterogeneous only very near the boreholes. Large geologic structures were implemented deterministically; the fractured bedrock was represented as an effective porous medium with relatively high permeability. Near the boreholes, background rock properties were used, with fractures that intersected the boreholes implemented as thin discrete features. The bentonite was modelled using both hydrogeological (H) and coupled hydrogeological-mechanical (HM) representations. In particular, the gap between the bentonite and the deposition hole wall was included in the HM model, allowing for the simulation of bentonite swelling.

2.8.3 Task 8A

Task 8A was simulated for a base-case parameter set and a number of sensitivity cases in which the rock and bentonite conductivities, the fracture transmissivity, retention parameters, and porosities were varied. It was concluded that background rock and bentonite permeabilities were the most relevant parameters. This result was partly a consequence of the fact that the fracture provided sufficient water (i.e. re-saturation is limited by the bentonite permeability), and that a large area of the deposition hole was in contact with the background rock.

2.8.4 Task 8C

Task 8C was modelled using 1) a full-scale, three-dimensional low-resolution model of the entire model domain, from which the results were used as boundary conditions for 2) a local, three-dimensional high-resolution model, only including one deposition borehole and the nearby fractured rock. Properties of the far-field effective continuum were taken from the calibration of a model of the prototype repository. Transmissivities of the fractures intersecting Boreholes KO0014 and KO0017 were calibrated to match the observed inflows and head distribution. Inflow into the widened surrogate deposition hole was then predicted using the calibrated model. Bentonite re-saturation with two background rock permeabilities was simulated, and the impact of an impermeable bottom plate was examined (Figure 2-54). It was concluded that the background rock permeability had a significant impact on wetting times.

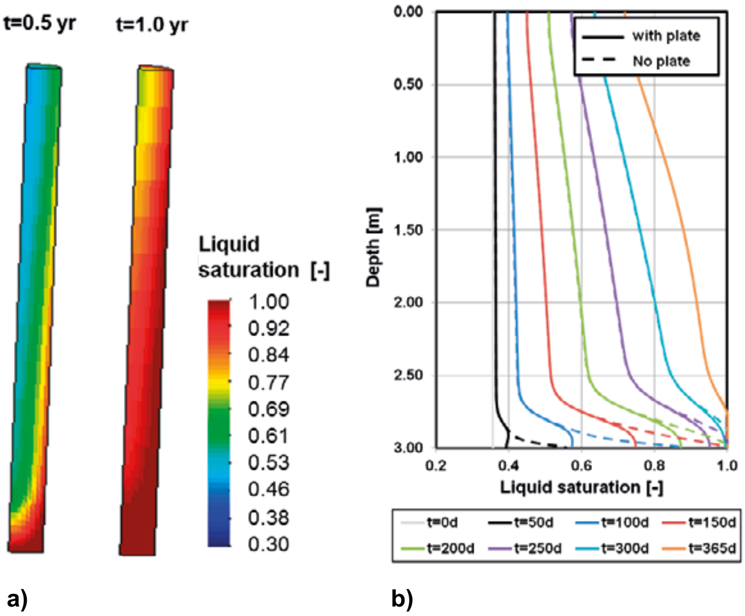


Figure 2-54. *Buffer saturation a) after 0.5 and 1.0 years, and b) vertical saturation profiles at eight different times (from Malmberg and Åkesson 2018).*

2.8.5 Task 8D/F

Tasks 8D and 8F were addressed concurrently (by including some dismantling data during model development for Task 8D). A single model was used that covered the far-field domain, local-scale region around deposition holes, and the bentonite (Figure 2-55).

The model, which was calibrated against available data (including some relative humidity measurements taken after dismantling), reproduced the observed inflows into the two boreholes KO0017 and KO0018 very well and the larger-scale pressure distribution reasonably well. After adjusting the sensor position relative to the location of the fracture intersecting the borehole (based on the actual orientation determined from excavation data), the observed and calculated relative humidity and water contents in the bentonite agreed reasonably well (Figure 2-56). Also, in order to account for the initial flooding of the borehole, which effectively led to a different initial suction without changes in water content, alternative retention curves were examined, which further improved the fit to relative humidity data.

2.8.6 Water-uptake test

The water-uptake test (WUT), was simulated using alternative models for the water retention and relative permeability functions, and compared to the measured saturation, relative humidity curves, and cumulative water-uptake volumes (Figure 2-58). The impact of an initial gap was also evaluated using the HM model. The analyses indicated that the initial gap can be neglected when modelling the field experiment, and that the parameters used to characterize the hydrogeological properties of the bentonite were suitable for numerical predictions of re-saturation.

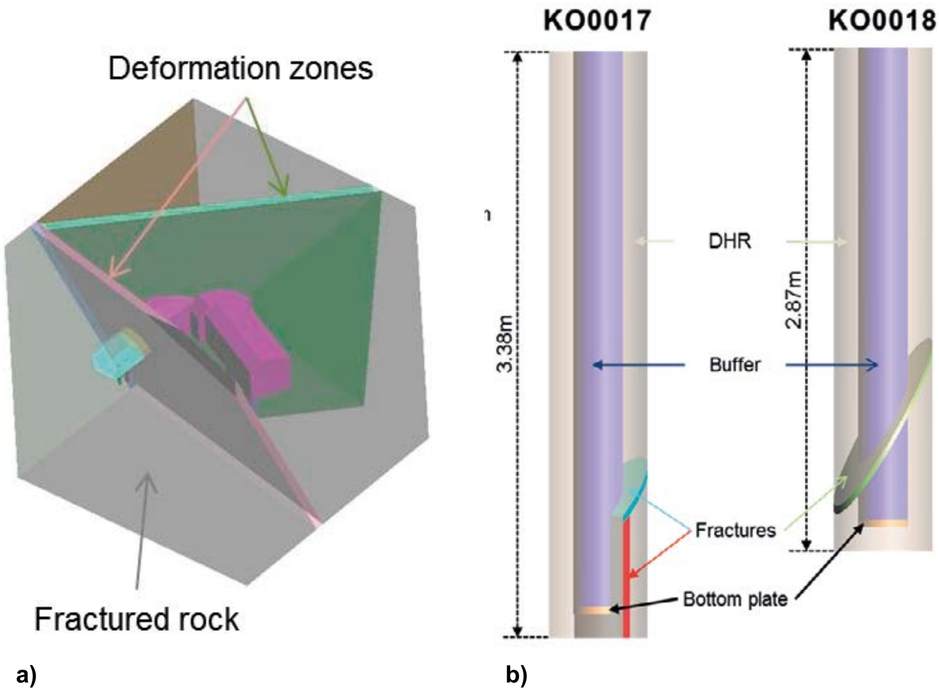


Figure 2-55. *a) Model domain and discrete fracture zones, and b) deposition holes with deterministic near-field fractures (from Malmberg and Åkesson 2018).*

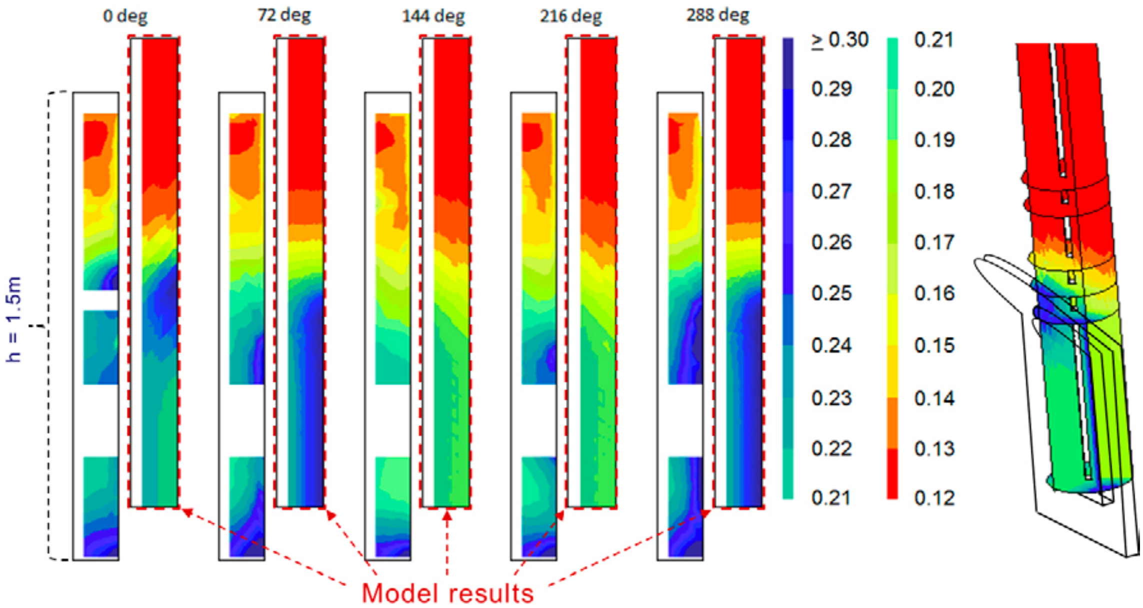


Figure 2-56. *Contour plots of the water content in Borehole 17 at the time of dismantling compared with experimental data (from Malmberg and Åkesson 2018).*

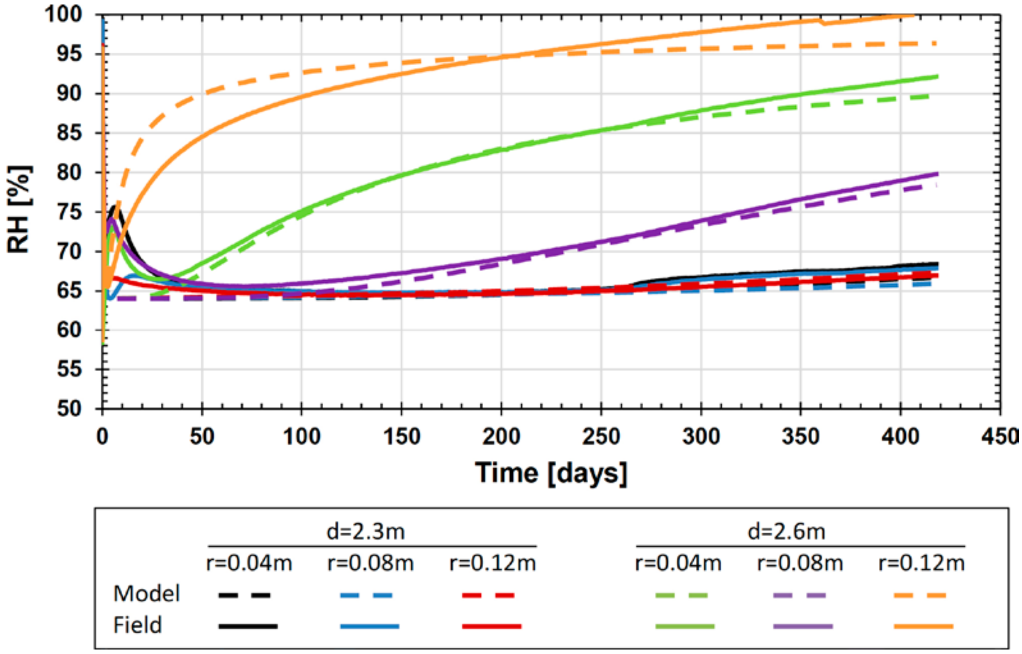


Figure 2-57. Relative-humidity evolution in Borehole 17 with an alternate retention curve and higher initial relative humidity (from Malmberg and Åkesson 2018).

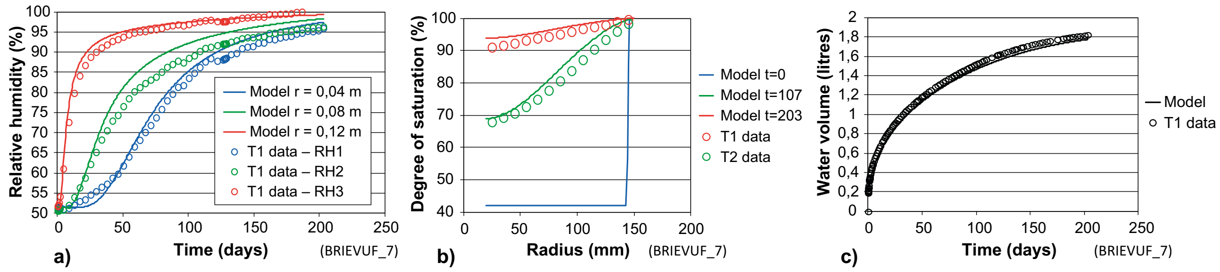


Figure 2-58. Water-uptake test; a) relative humidity, b) water saturation, and c) cumulative water-uptake (from Malmberg and Åkesson 2018).

2.8.7 Concluding remarks

The following conclusions were drawn from the simulation of the water-uptake laboratory experiment and the modelling of the BRIE field experiment:

- The initial gap between the bentonite and the deposition hole wall can be ignored when analyzing the wetting of the bentonite in BRIE because of its small width and since it was initially filled with water.
- The hydraulic parameters from the task description are reasonable and can be used for predicting bentonite re-saturation under field conditions.
- Uncertainties in the contribution of background rock flow to the bentonite wetting in BRIE was reduced by measuring the relative humidity evolution at several different positions in the bentonite.
- Background rock permeability appears to be low at borehole KO0017, i.e. re-saturation is dominated by fractures intersecting the deposition hole.
- Background rock permeability, number and properties of intersecting fractures, as well as bentonite permeability are the key factors affecting bentonite re-saturation.

2.9 Modelling group: SKB-KTH

2.9.1 Introduction

The Task 8A modelling work performed by the Royal Institute of Technology (KTH), Stockholm, Sweden, is documented here.

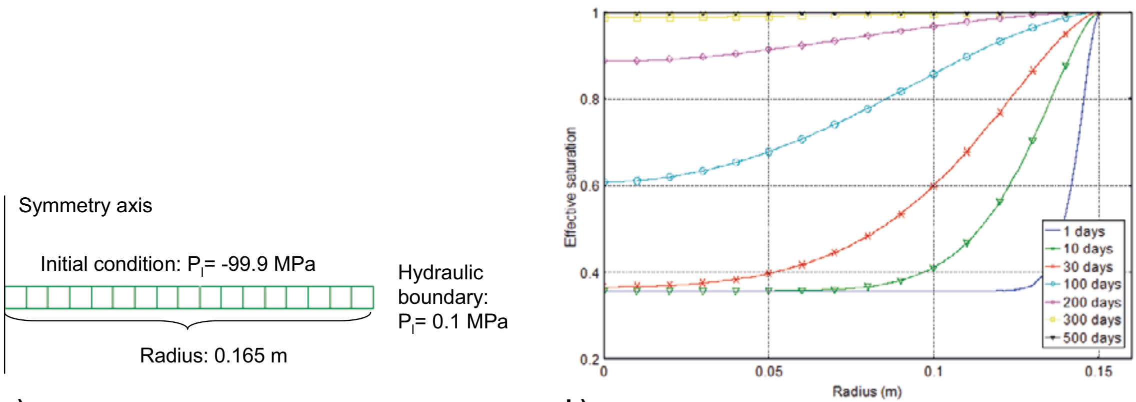
2.9.2 General modelling approach

A code was developed that can handle saturated and unsaturated flow using a pressure formulation of the Richards equation in which the accumulation term uses the specific moisture capacity and storage coefficient to capture time-dependent volumetric fluid changes under both saturated and partially saturated conditions. The coefficients in the equation were reformulated to be easily related to parameters of water flow through a fracture (rather than porous medium). Task 8A was used as a code verification case.

2.9.3 Task 8A

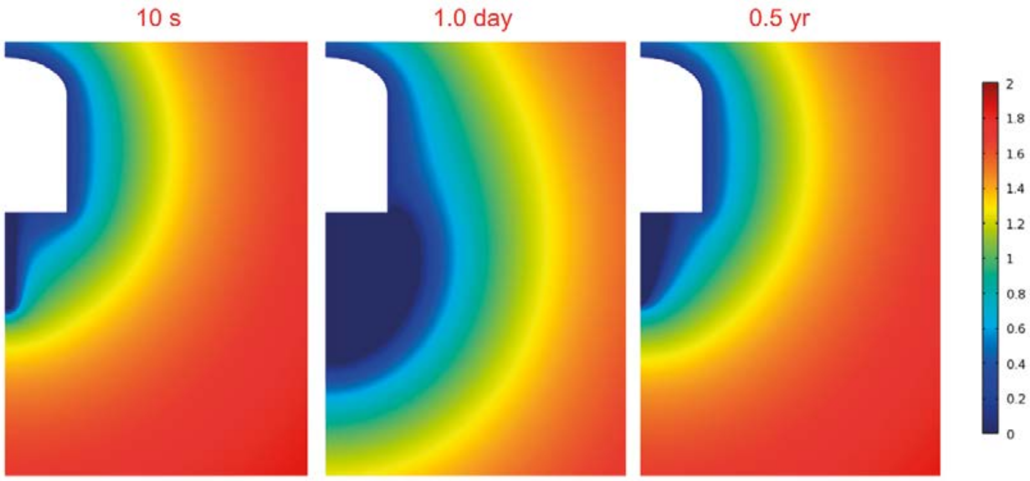
A radial homogeneous model was developed to simulate bentonite re-saturation from the outside (Figure 2-59).

The Task 8A configuration with and without a horizontal fracture was simulated, whereby the fracture was either represented as a 0.1 m thick porous medium of high permeability, or as a discrete fracture of 0.1 mm aperture and appropriate transmissivity and storativity values. While the presence or absence of a fracture clearly affected pressure and flow distribution as well as the bentonite re-saturation time, the differences obtained with the two alternative fracture representations were insignificant except at very early times (Figure 2-60).

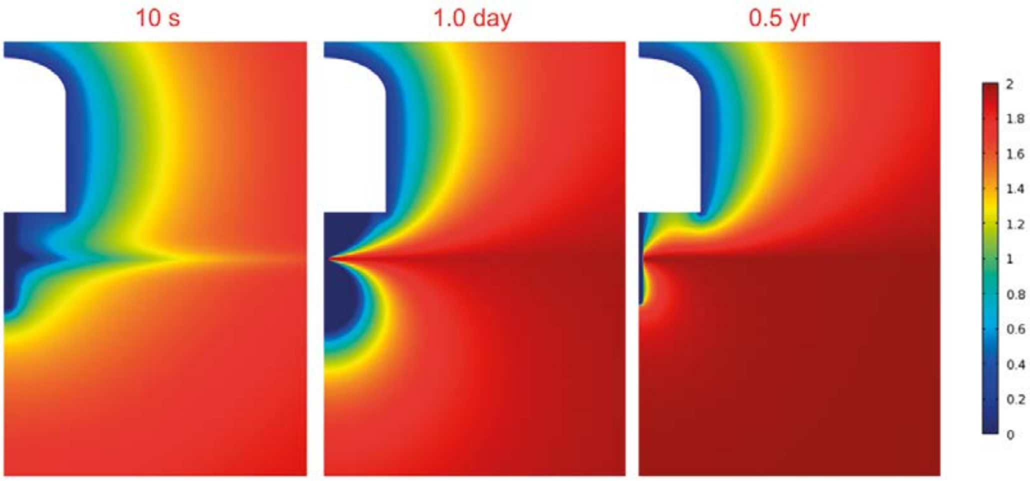


a) b)

Figure 2-59. a) Axi-symmetric model setup and b) radial distribution of water saturation.



a)



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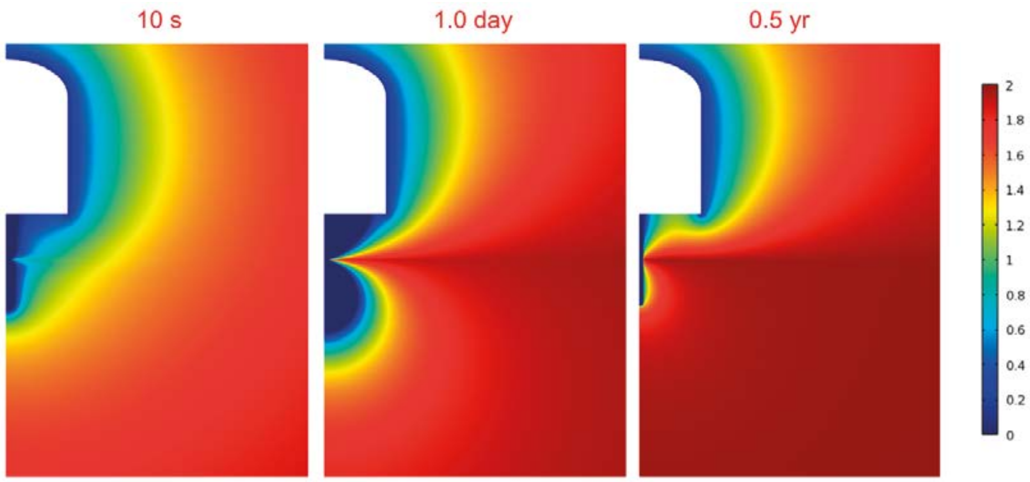


c)

Figure 2-60. *Pressure distribution a) without a fracture, b) with a 0.1 m thick high-permeability porous layer, and c) a 0.1 mm discrete fracture.*

2.10 Modelling group: SKB-SU

2.10.1 Introduction

The Task 8A–D modelling work performed by the Swedish Nuclear Fuel and Waste Management Company (SKB) and Stockholm University is documented in Dessirier et al. (2017). The modelling work focused on the determination of the effects of fractures and heterogeneity on two-phase air-water flows in the near-canister domain and the assessment of the extent of sub-grid scale processes (e.g. bubble trapping, gas dissolution) both in the bentonite buffer and the natural, sparsely fractured bedrock.

2.10.2 General modelling approach

The approach consisted of examining different scenarios to evaluate conceptual assumptions about the impact of the gas phase on bentonite re-saturation. Specifically, the simplified Richards equation approach was compared to a multi-phase formulation in which the gas phase was explicitly accounted for, allowing for phase-change and trapping effects. Moreover, different scenarios regarding the location of fractures intersecting the boreholes were investigated. The TOUGH2 code (Pruess et al. 1999) was used for the analyses.

2.10.3 Task 8A and global sensitivity analysis

Re-saturation of the bentonite was examined for different scenarios regarding fracture position and the explicit inclusion of a gas phase. Systematic differences between a modelling approach based on Richards' equation and a full two-phase formulation were observed, where the former led to shorter re-saturation times (Figure 2-61). The impact of gas relative permeability and air diffusion was evaluated, as it affects advective and diffusive transport (potentially reaching boundaries such as the TASO tunnel) as well as air dissolution in the liquid phase. The model also predicted considerable desaturation of the background rock around the deposition hole. The amount and fate of dissolved air was considered important as it may affect bio-geochemical reactions and corrosion rates.

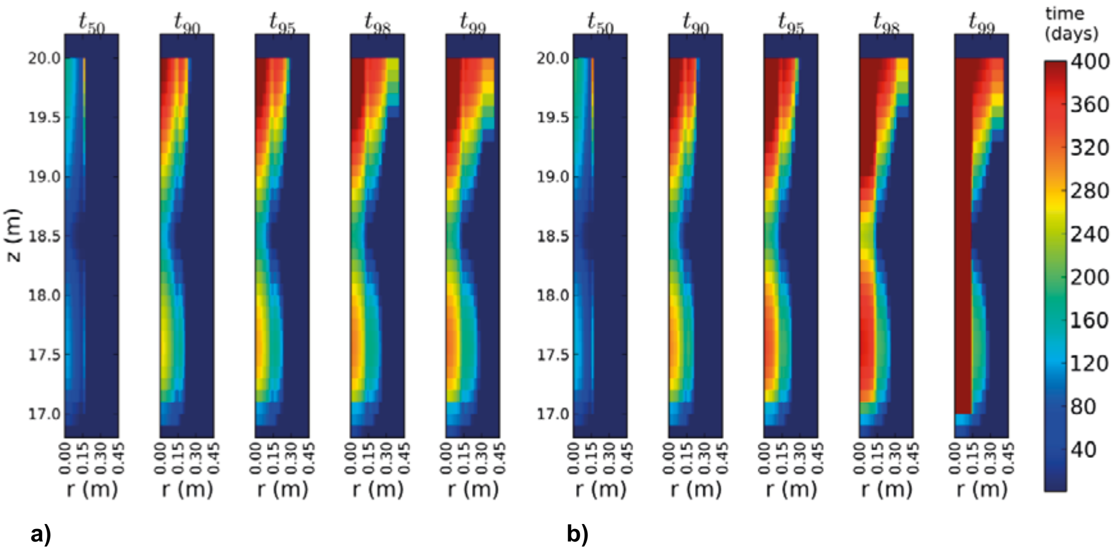


Figure 2-61. Times to reach defined percentages of saturation using a) Richards' equation, and b) two-phase formulation (from Dessirier et al. 2017).

A global sensitivity analysis was performed to identify influential parameters with respect to three predictions of interest: 1) the saturation time in the buffer, 2) re-saturation time of the rock wall, and 3) the amount of air initially introduced with the buffer that undergoes dissolution into the liquid phase. The Morris method was applied to examine the mean elementary effect (μ*) and standard deviation (σ) derived from sensitivities evaluated at multiple points in the admissible parameter space. As an example, Figure 2-62 shows the cumulative density function (CDF) and sensitivity measures of the time required to nearly (> 95 %) saturate 75 % of the buffer. The time needed to nearly saturate 75 % of the installed buffer ranges approximately from 100 to 10 000 days with a median around 300 days. The statistics of the elementary effects are represented by the points in the (μ^*, σ) plane and their associated uncertainty bars corresponding to a confidence level of 95 % estimated by resampling. The parameters with highest sensitivity (placed near the top right of the figure) include permeability of the background rock, the outer boundary pressure, the ventilation-induced suction at the tunnel wall, and the position of the fracture. None of the parameters can be clearly excluded as being non-influential, indicating that the saturation time of the buffer is a prediction with a complex sensitivity structure due to a high number of influential parameters with non-linearities and/or parameter interactions.

The following conclusions were drawn from the Task 8A modelling study:

- The installation of a bentonite buffer can cause considerable desaturation of the adjacent background rock (later corroborated by relative humidity measurements).
- The position of the fracture / deposition hole intersection can considerably influence re-saturation times.
- Whereas 95 % saturation is reached within two years in the considered cases, considerably longer times are needed to reach 99 % saturation.
- Richards' equation systematically predicts higher degrees of saturation and shorter re-saturation times than the model with full two-phase flow representation.
- The under-prediction of re-saturation time made by Richards' equation increases substantially as the system approaches full saturation.
- A considerable amount of gas may dissolve into the relatively immobile liquid phase and remain in the vicinity of the deposition hole for an extended period.
- The global sensitivity analysis revealed that each model prediction may span a wide range, and that the sensitivity structure is complex, i.e. the predictions are highly sensitive to a relatively large number of parameters, and there are significant parameter interactions and/or non-linearities.
- It is difficult to reduce the number of model parameters necessary to predict the time to buffer saturation.

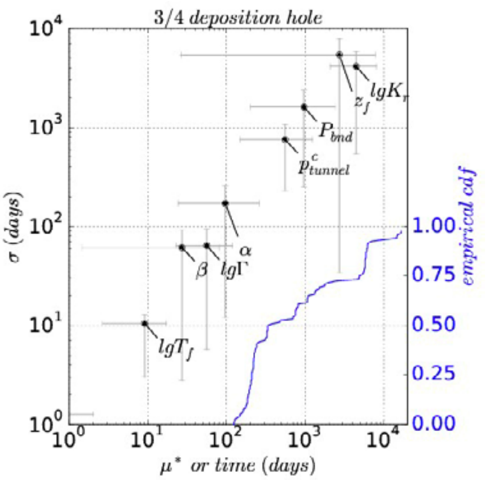


Figure 2-62. *Empirical cumulative density function (blue line, right axis) and elementary effect distribution in the (μ*, σ) plane for the time to nearly saturate 3/4 of the inserted buffer (from Dessirier et al. 2017).*

2.10.4 Inflow into openings

A three-dimensional model with various skin zones around openings was developed to simulate inflow into tunnels and boreholes. The dominant fractures intersecting the deposition holes were explicitly included into the model (Figure 2-63). Three scenarios were formulated, reflecting different assumptions about permeabilities and accessibility to structural information. Each scenario was calibrated against inflow data to determine background rock permeability and/or fracture transmissivities.

2.10.5 Bentonite re-saturation

The three calibrated models were used to simulate bentonite re-saturation. They were compared to data from the relative humidity sensors placed in the bentonite; a subset of the results is shown in Figure 2-64. It was concluded that information about the location of key fractures intersecting the deposition holes (if they exist) was more relevant than assumptions about the properties of these fractures or the background rock.

Simulations of rock de-saturation after bentonite emplacement (and discrepancies to the observed slow re-saturation) suggested that two-phase characteristics of the rock might not have been properly captured.

The following conclusions were drawn from the modelling of BRIE:

- The understanding of the main structural features contributing to bentonite water-uptake remains limited. Heterogeneity of the rock mass has a strong regulating effect on the flow rates observed during bentonite wetting.
- Detailed information on the location of inflow points and traces seems more effective to constrain the predictions of wetting time than open-hole aggregated inflow rate measurements.
- Analyses of dismantled rock wall samples revealed a lack of understanding of the re-saturation dynamics in the rock wall.
- It is recommended to include spatial inflow point characterization into the criteria used to assess the fitness of a potential deposition hole.

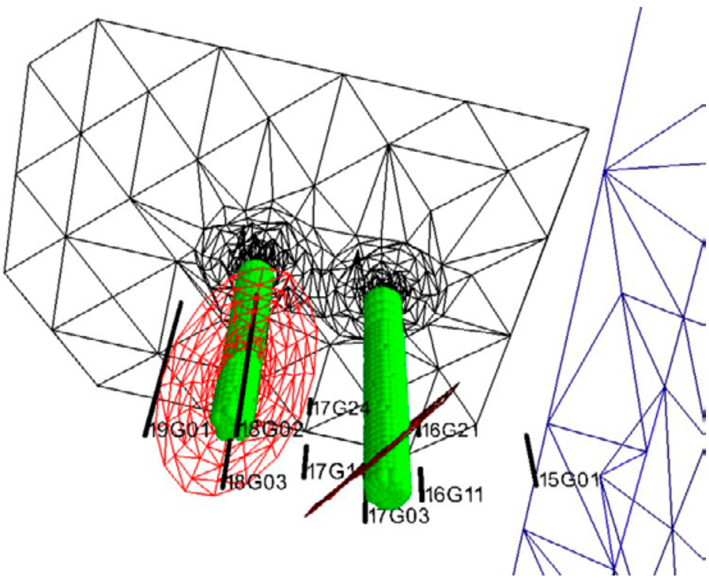


Figure 2-63. *Model geometry in the floor of the BRIE tunnel: deposition holes (green), local fractures (red), large geologic structure (blue), borehole intervals and tunnel floor (black) (from Dessirier et al. 2017).*

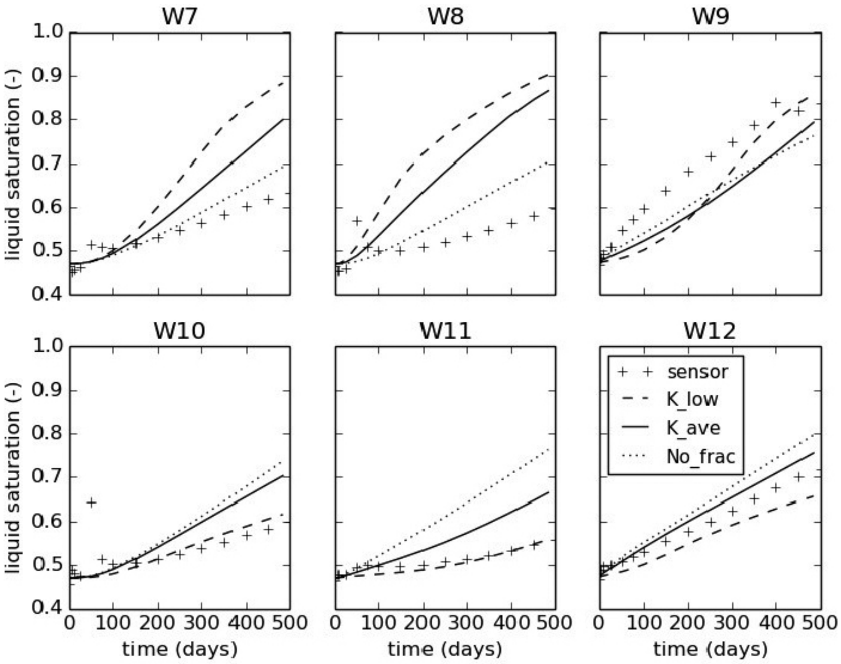


Figure 2-64. Liquid saturation history inferred from relative humidity sensors W7–W12 and from modelling scenarios (from Dessirier et al. 2017).

2.10.6 Bentonite photograph analysis

A quantitative reconstruction of the water content from photographs of the dismantled bentonite surface and from water content sampling (Figure 2-65) was developed to better assess the relative importance of inflow features and thus help constrain numerical models. A correlation between surface sample and greyscale values was used in combination with geostatistical interpolation of the residual to arrive at maps of reconstructed gas saturation distributions and associated uncertainties (Figure 2-66). The regression-kriging procedure applied to the dismantling photographs captured more features influencing the groundwater inflow at the bentonite/rock interface than traditional interpolation methods based solely on points measurements. The results from the reconstruction also seemed to reveal information on the in-plane channelling in the fracture as well as vertical conductive features possibly related to stress effects.

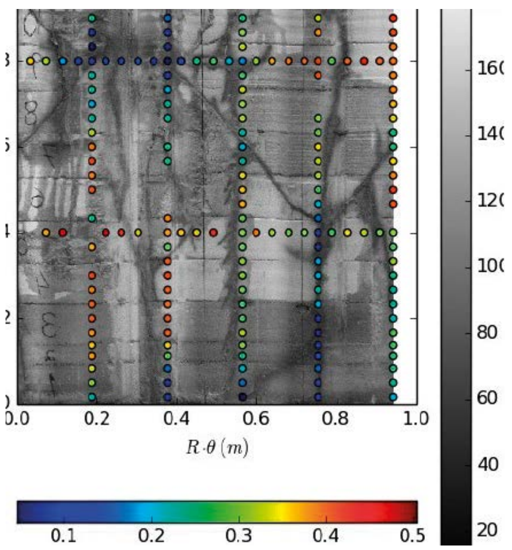


Figure 2-65. Overlay of the assembled panorama of grey scale unfolded surface elements retrieved from dismantling photographs (background) and translated gas saturation from measurements on samples (coloured dots) (from Dessirier et al. 2017).

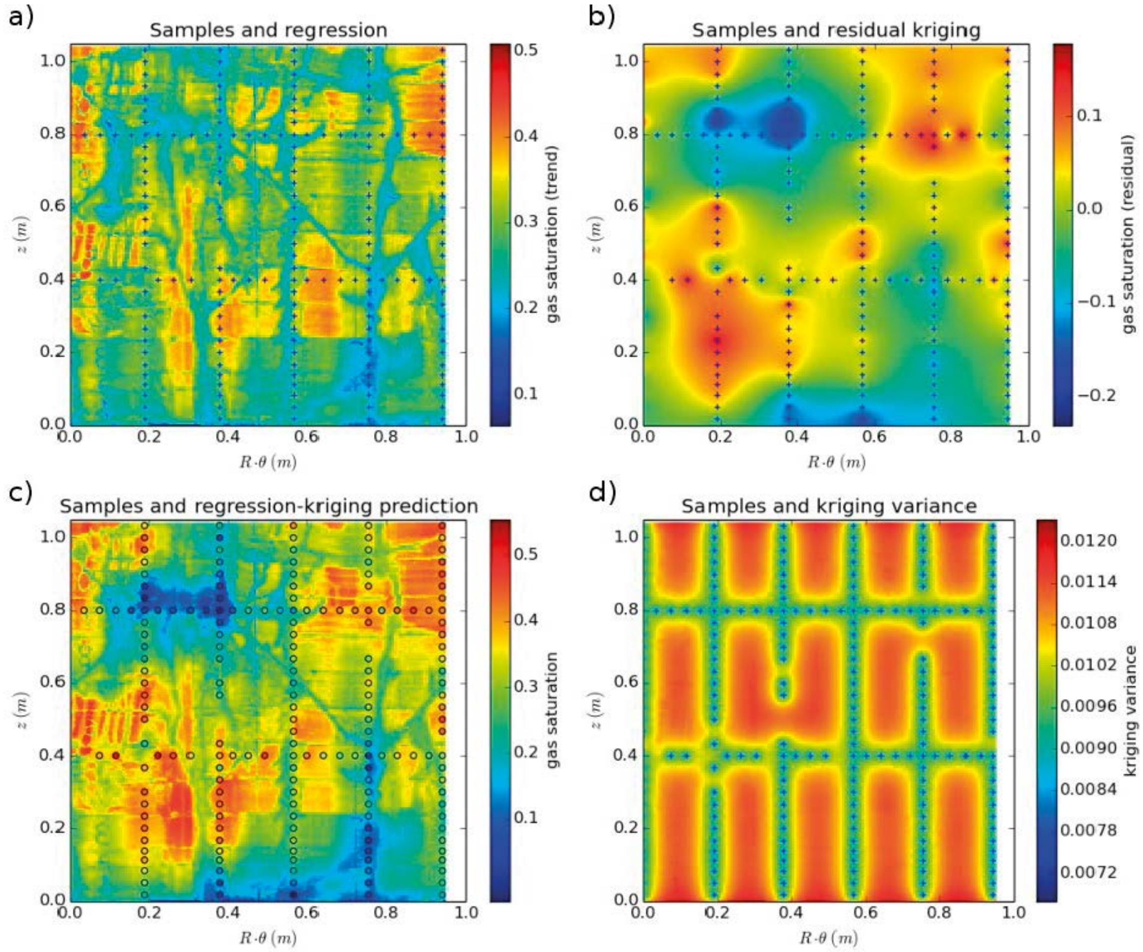


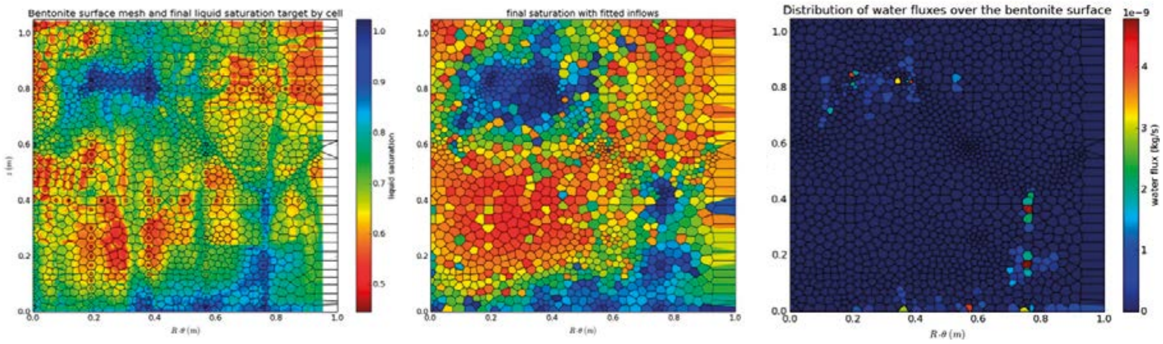
Figure 2-66. *Unfolded bentonite surface reconstruction of gas saturation by regression-kriging: a) regression, b) kriging of residuals, c) regression-kriging prediction, and d) kriging variance (from Dessirier et al. 2017).*

2.10.7 Reproduction of water inflow distribution

The surface saturation map derived from the unfolded bentonite surface reconstruction of Borehole 18 was inverted to 1) derive the inflow distribution at the bentonite-rock interface and compare it to the lumped inflow values obtained previously during the deposition hole characterization, and 2) assess the quality of the reconstructed final saturation by comparing the saturation resulting from the estimated inflow distribution to the saturation response observed at six sensors.

A local, cylindrical model of the lower part of Borehole 18 was developed. Inflow rates for the highest 230 saturation points were estimated in a series of sequential inversions, and eventually all (1 428) rates were estimated in a joint inversion. The resulting inflow and corresponding saturation distributions are shown in Figure 2-67.

The sum of all inflows was compared to the measured inflow into open holes, and the resulting saturation distribution was compared to the time series of saturations from the relative humidity sensor (data not used for the inversion); see Figure 2-68.



a) b) c)

Figure 2-67. Unfolded bentonite surface map of a) target saturation, b) simulated saturation, and c) estimated inflow distributions (from Dessirier et al. 2017).

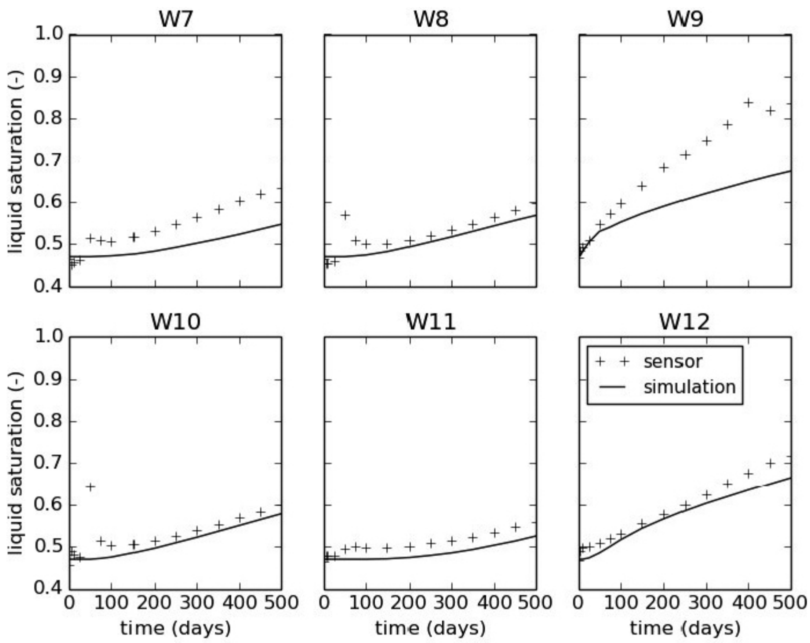


Figure 2-68. Comparison of measured and modelled sensor responses as a function of time (from Dessirier et al. 2017).

2.10.8 Conclusions, open issues, and recommendations

The following overall conclusions and recommendations were made:

- The installation of a bentonite buffer can cause considerable de-saturation of the adjacent background rock.
- The position of the fracture(s) / deposition hole intersection(s) can considerably influence buffer saturation times.
- The aggregated open deposition hole inflow value does not help significantly constrain the buffer wetting time without information on the spatial distribution of the inflow points.
- Richards' equation systematically predicts higher degrees of saturation and shorter re-saturation times than the model with full two-phase flow representation. The under-prediction made by Richards' equation increases as the system approaches full saturation.
- A significant part of the gas initially present in the bentonite may dissolve into the relatively immobile liquid phase and remain for decades or more in the vicinity of the deposition hole.
- An attempt to infer a quantitative inflow map from an inversion of the bentonite surface saturation map yielded plausible results.

Open issues of potential significance were identified. They include:

- Occurrence and impacts of de-saturation of the rock domain in the near-canister region.
- Possible effects of (uncertain) background fracture networks and statistics and the effect of in-plane channelling/fracture roughness.
- Influence of biological and geochemical processes on residence times of air dissolved in water.
- Possible questioning of the concept of intrinsic permeability for bentonite.
- Uncertainties in estimating time to full re-saturation.

The following recommendations were made:

- Additional scenario-based, stochastic uncertainty analyses should be performed in order to investigate the time scales for buffer re-saturation and potential transport pathways from the rock to the bentonite.
- Attention should be paid to detailed modelling of two-phase flow dynamics in the near-canister domain, as neglecting two-phase flow dynamics adds significant uncertainty in the estimated times to buffer saturation.
- The geometry of the fracture / deposition hole intersections should be considered as a deposition hole siting criterion.
- The ultimate fate of the air included in the bentonite should be investigated, as it may significantly impact biogeochemical processes.

2.11 Modelling group: Technical university of liberec

2.11.1 Introduction

The Task 8 modelling work performed by the Technical University of Liberec, Czech Republic, is documented in Hančilová and Hokr (2018), which describes the modelling of Subtask 8A, the prediction of bentonite wetting within Task 8D, and a sensitivity study of inflow into the borehole under saturated conditions.

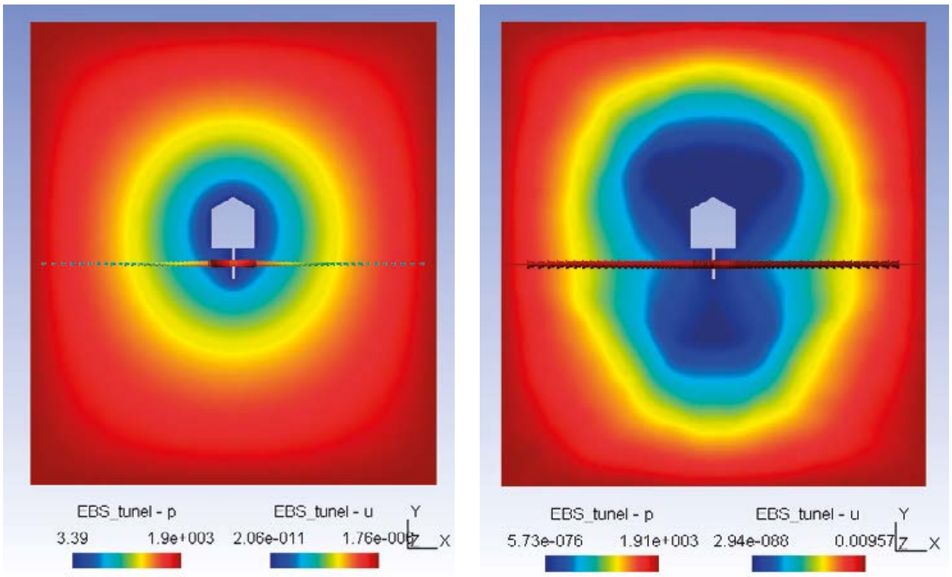
2.11.2 General modelling approach

Fluid flow in the geosphere and inflow into the open borehole was modelled assuming fully saturated conditions using the code Flow123D, which is a mixed-hybrid finite element code that allows 1D and 2D elements to be embedded into a 3D computational grid. Bentonite re-saturation was analysed using a diffusion equation approach. This is equivalent to solving Richards' equation with a nonlinear (hydraulic) diffusivity; however, saturated conditions cannot be addressed. The code Ansys was used for this analysis.

For the modelling of bentonite re-saturation, the fracture rock was not included; instead, constant pressure (Dirichlet) boundary conditions were specified at fracture intersection trace lines, and specified flux (Neumann) boundary conditions were applied where the bentonite is in contact with the background rock.

2.11.3 Initial sensitivity analysis

An initial sensitivity analysis using a 2D model was performed to evaluate the relative importance of fracture and background rock inflow into an open borehole assuming fully saturated conditions. Figure 2-69 shows the pressure distribution for different ratios of fracture and background rock permeability. The corresponding inflows into a deposition hole were recorded.



a) b)

Figure 2-69. *Pressure fields (colour scale) and velocities (arrows) for a) high background rock and low fracture permeabilities, and b) low background rock and high fracture permeabilities (from Hančilová and Hokr 2018).*

2.11.4 Task 8A

The Task 8A scenario was simulated for linear and radial configurations using the diffusion form (with a nonlinear hydraulic diffusivity) of the Richards equation. The results are compared to the solution provided in the task description (Vidstrand et al. 2017). To better reproduce this solution, rock permeability was significantly reduced (by a factor of 67), whereas bentonite permeability was increased (by a factor of 1.5).

2.11.5 Task 8D

Bentonite re-saturation was simulated using a conceptual model in which the fractured rock was not explicitly modelled; instead, constant pressure (Dirichlet) boundary conditions were applied at fracture intersection trace lines, and constant flux (Neumann) boundary conditions where the bentonite was in contact with the background rock. This conceptual model was exercised with and without accounting for the influence of the background rock, and using different fracture trace maps. The various simulations showed the influence of the number, location, and trace lengths of fracture intersections, and the impact of inflow through the permeable background rock. An example is shown in Figure 2-70, with comparisons to relative humidity data depicted in Figure 2-71.

2.11.6 Water-uptake test

The water-uptake test was simulated using the same modelling approach, whereby the nonlinear hydraulic diffusivity was calculated for different assumptions about the water retention and relative permeability curves. All variants matched the observed cumulative water-uptake volume equally well. Some differences were visible when comparing saturation or relative humidity profiles.

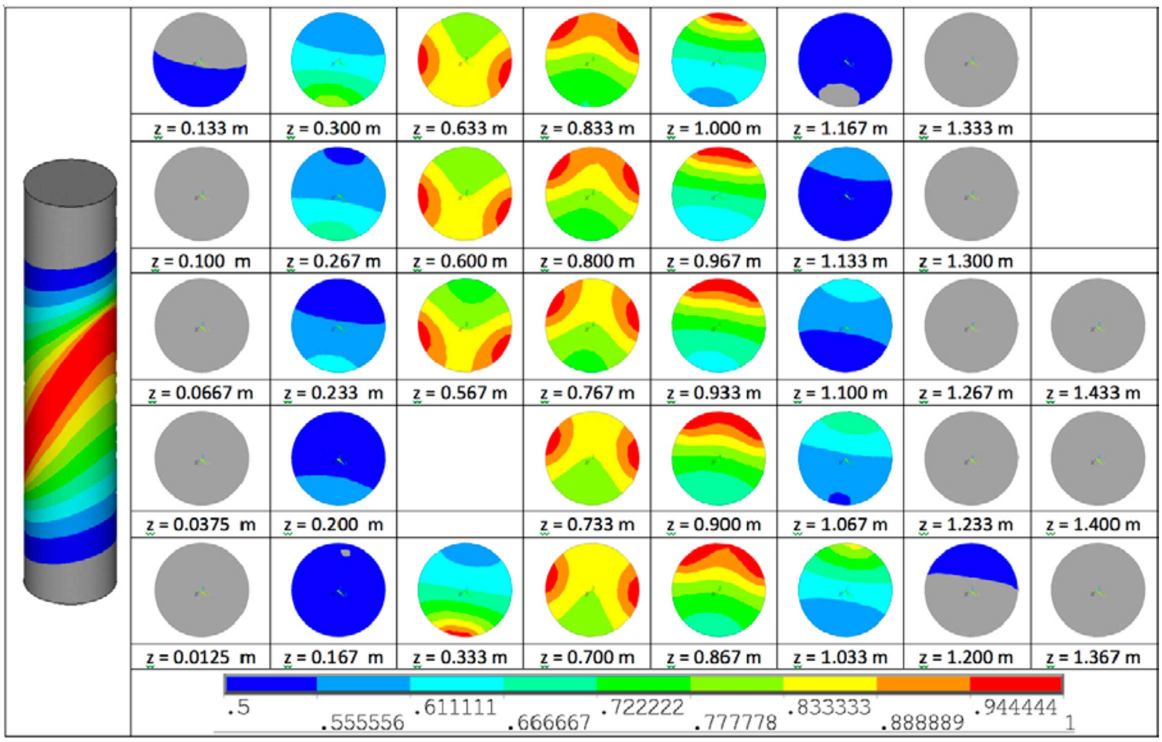


Figure 2-70. Cross sections of simulated saturation distributions for bottom part of borehole KO0017G01 (from Hančilová and Hokr 2018).

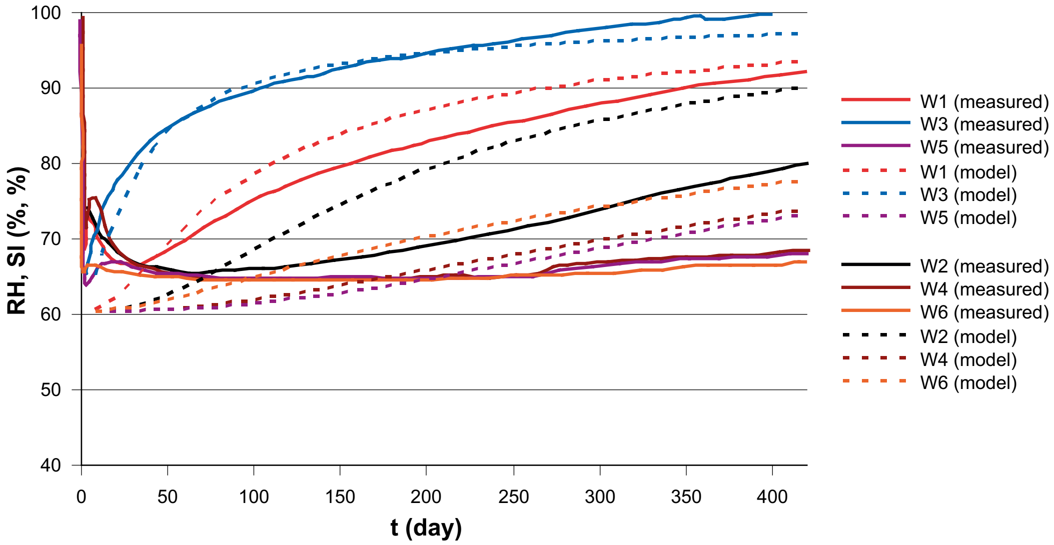


Figure 2-71. Comparison between measured and simulated relative humidities in borehole KO0017G01 (from Hančilová and Hokr 2018).

3 Review and evaluation of modelling work

3.1 Introduction

Chapter 2 is an attempt to condense the modelling groups' interpretations, conclusions, and recommendations without an evaluation. Chapter 3 summarizes some of the specific review comments made by the evaluator. Detailed review comments and the modelling groups' responses are documented in SKB "Review Statement/Response Statement" forms, which are considered an integral part of the Task 8 evaluation. Some of these review comments have been communicated to the modelling groups prior to the writing of this evaluation report, i.e. they were discussed throughout the course of Task 8. They were based on draft reports and presentations made during the various Task Force meetings. Some of the review comments were addressed and are reflected in the final reports.

In the following subsections, some general remarks are given that relate the accomplished work to the main objectives, as stated for each subtask in the task description (Vidstrand et al. 2017; see also Section 1.5); the objectives are restated below in italics. Review comments and evaluations are documented for each modelling group individually. An overall evaluation of Task 8 can be found in Chapter 5.

It should be noted that the work of the modelling groups was sponsored by their respective organizations. The amount of time, funding, personnel, and other resources available to work on Task 8 likely varied considerably among the participating modelling groups. This difference in available resources is acknowledged, but could not be explicitly accounted for in this evaluation report.

3.2 Modelling group: GRS

Section 2.1 summarizes the work and interpretation of GRS as described in the project report Kröhn (2017, 2018). Technical review comments are documented in the related SKB Review Statement.

Task 8A

Did the work identify a suitable method for incorporating bentonite in numerical groundwater flow models, and was the effect of different implementations of the bedrock-bentonite interface evaluated? Did the work provide insights regarding the importance of fractures?

GRS opted to skip Task 8A. It would have been an opportunity to describe the chosen approach of separating the problem of groundwater flow in the fractured bedrock from that of bentonite wetting. The two cases of Task 8A (inflow through background rock only or with a fracture embedded) would have alerted GRS early on that the VIPER code could not handle the case of restricted water supply at the bedrock-bentonite interface.

Task 8B

Did the work identify a suitable method for incorporating unsaturated, fractured rock and to examine effects of different concepts, boundary conditions, and properties on bentonite re-saturation?

The work demonstrated that the d^3f code is a powerful tool capable of simulating steady-state, saturated groundwater flow in systems with discrete features embedded in porous material. The code can also represent complex geometry and boundary conditions. The question of unsaturated flow has not been addressed, not only because it is beyond the code's capabilities, but also mainly because the one-way coupling between the natural and engineered barrier systems did not allow to consider feedback mechanisms (e.g. the strong suction of the bentonite) that could potentially create partially saturated conditions.

The impact of the large discrete geologic structures on the inflow distribution to the underground openings was examined, revealing the importance of the boundary conditions, but also the relative minor influence of these features on small-scale flow patterns. The lack of calibration data was cited as a limitation; this shortcoming could have been partly addressed by performing systematic sensitivity and uncertainty analyses.

Task 8C

Did the work predict inflows and inflow characteristics to surrogate holes, and examine the importance of deformation zones and fractures on bentonite re-saturation?

The main outcome of this task was the insights gained by the attempt to calibrate the model. It was concluded that the effects of the large geologic structures were essentially insignificant, and that the proposed conceptual model could not capture variability in the inflows to probing holes unless *ad hoc* artificial fractures were introduced. The decision to make the background material (which represents the background rock and smaller fractures) homogeneous may have contributed to the lack of inflow variability. The model matched the observed inflows within a factor of four; it appears that this match is considered acceptable; a related discussion would be useful.

Task 8D

Did the work predict inflows and inflow characteristics to open probing and surrogate deposition holes and examine the impact of fractures and heterogeneity in fractures and matrix on bentonite re-saturation?

The conceptual model was changed by introducing skin zones around all underground openings. While the motivation for this adjustment was described, it did not resolve the fundamental issue of how to generate inflow characteristics that are similar to the observed flow distributions. Nevertheless, a range of inflows (from the background rock and fractures) was used as boundary conditions for the bentonite wetting model. Confidence in the bentonite model was gained by thee term comes from SKB good reproduction of the water-uptake test. A classification of "restricted" and "unrestricted" water supply was proposed, where only the former shows any significance of the bedrock hydraulics on bentonite wetting. Defining these two modes was useful and helped clarify which aspects of the system need to be characterised. It should be recognized, however, that this categorisation neglects the feedback of the bentonite on the bedrock (e.g. pressure build-up and thus increased driving force in the unrestricted case, and capillary pressure gradient and desaturation in the restricted case); the one-dimensionality of the VIPER model also prevented the analysis of heterogeneous wetting distributions and three-dimensional effects on wetting time.

Task 8F

Did the work predict inflows and bentonite wetting characteristics that were consistent with the data collected during the BRIE experiment, including the data obtained after dismantling? Did the work comment on the validity of the initial hypotheses and conceptual models in the light of the available BRIE data?

The initial hypotheses and conceptual model decisions were examined by an extensive discussion of the available BRIE data (specifically those obtained by dismantling the bentonite in Boreholes 17 and 18). Model assumptions and code limitations were assessed and critically reviewed. Final simulations were performed with the existing tools for subproblems that fit the assumptions and model capabilities. Remaining inconsistencies were presented, and the range of applicability and limitations of the approach and tools were discussed. The conclusions drawn from Task 8F significantly contributed to the overall insights gained by GRS for the entire Task 8 project.

Overall

Did the work improve the scientific understanding of the exchange of water across the bentonite-rock interface, and help better predict the wetting of the bentonite buffer? Did the work improve the characterisation methods of the canister boreholes and help establish deposition hole criteria?

The modelling of Task 8 documented in Kröhn (2017) improved the understanding of certain features of the natural system on the performance of the engineered barrier. The chosen modelling approach, specifically the separation of the groundwater and bentonite re-saturation models, is probably useful and acceptable for the intended use of these models; however, it would have been preferred if the appropriateness of this approach were demonstrated by comparing it to the results of a model in which the two systems were fully coupled, thus accounting for feedback mechanisms. The proposed classification of bentonite wetting under restricted and unrestricted water supply conditions – each with its distinct re-saturation behaviour – can be considered a screening method for deposition hole characterisation.

GRS described the process of hypothesis formulation, model development, data analysis, and result interpretation in great detail. The availability of new data from BRIE and of modelling results led to a constant evolution of the model that tested hypotheses and yielded considerable insights. While GRS decided early on to separate the fractured rock model from the bentonite wetting model using different software tools (d^3f and VIPER, respectively), the details within and interaction between the two subproblems were continuously examined; adjustments were made to both the conceptual model and the code as needed.

For the bedrock, the role of fractures (both the deterministically defined large geologic structures and the stochastically described smaller fractures as well as uncharacterized microfractures) was examined and led to a model progression in which the initially unaccounted fracture network was then represented by a homogeneous rock mass of increased permeability, whereby the region around the deposition holes was treated separately (and, later, a skin zone was introduced around all geotechnical openings). Next, the need for introducing artificial, discrete fractures was recognized to establish connectivity, but led to further adjustments of the rock-mass properties that were considered unreasonable. Observed variability in inflow on the borehole scale (and eventually bentonite wetting patterns) finally led GRS to conclude that a deterministic treatment is inappropriate, and that a stochastic approach prevents one from making specific predictions about the suitability of individual deposition holes.

Bentonite wetting was separated into two scenarios (restricted and un-restricted water supply), a classification that proved conceptually insightful and computationally useful within the limitations of the chosen approach to separate the geosphere from the engineered barrier system at the bentonite-rock interface. Predicting and reproducing data from the water-uptake test under idealized conditions yielded confidence in the representation of the bentonite. The model was then applied to the much more complex conditions and data from the dismantling of BRIE. However, GRS clearly outlined the limited range of applicability of their model, and avoided making unsubstantiated statements about their ability to accurately predict bentonite buffer wetting under realistic installation conditions.

The implications of the key modelling decisions (decoupling of model domains; dimensionality and processes used in each submodel) on results and conclusions could have been examined in more detail. However, the evolution of conceptual model understanding, modelling tools, and hypotheses, and the inclusion of information from BRIE into this process are exemplary.

In summary, GRS made substantial contributions to the understanding of the bentonite-rock interface, bentonite wetting, and the modelling process used to gain such understanding. The active participation and many contributions made during the Task Force meetings are very much appreciated.

3.3 Modelling group: JAEA

Section 2.2 summarizes the work and interpretation of JAEA as described in the project report Sawada et al. (2019). Technical review comments are documented in the related SKB Review Statement. The following are some remarks that relate the accomplished work to the main objectives. JAEA did not participate in Task 8A.

Task 8B

Did the work identify a suitable method for incorporating unsaturated, fractured rock and to examine effects of different concepts, boundary conditions, and properties on bentonite re-saturation?

The FracMan/MAFIC code was used to simulate saturated flow through a discrete fracture network, whereas Thames was used to simulate bentonite re-saturation based on Richards' equation. The proposed iterative scheme between the engineered and natural system partly accounts for feedbacks between the two systems. However, the scheme makes some unphysical (neglect of suction) or arbitrary choices (pressure head set to 5 m if saturated conditions exist). Considerable efforts were made to develop and implement this iterative coupling approach; careful testing of the assumptions made at the interface between the two submodels would have demonstrated the appropriateness of this conceptualization.

Only large water-conducting features were implemented in the model along with a single hypothetical fracture that intersects the deposition hole. Under these specific conditions, the effect of a single discrete inflow plane on the bentonite wetting time is demonstrated.

Task 8C

Did the work predict inflows and inflow characteristics to deposition holes, and examine the importance of deformation zones and fractures on bentonite re-saturation?

Inflows predicted by the DFNs varied considerably between individual realizations. However, the spatial variability of inflows observed in the field was not reproduced, suggesting that flow-controlling features or mechanisms are not fully captured by the stochastic DFN. Moreover, despite considerable characterization data on fracture geometry and correlations between fracture length and transmissivity, the observed rates were substantially over-predicted by the model, requiring calibration and model adjustment steps. Conditioning the DFN to water conducting features observed in the deposition holes appears a reasonable approach, but it was insufficient to significantly improve the predictions at this stage.

Task 8D

Did the work predict inflows and inflow characteristics to open probing and surrogate deposition holes and examine the impact of fractures and heterogeneity in fractures and matrix on bentonite re-saturation?

The flow and rewetting characteristics did not fundamentally change as a result of further conditioning of the model. This might have been an opportunity to revisit the assumptions and parameter choices, and to potentially make adjustments (both refinements or simplifications) to the conceptual model.

Task 8F

Did the work predict inflows and bentonite wetting characteristics that were consistent with the data collected during the BRIE experiment, including the data obtained after dismantling? Did the work comment on the validity of the initial hypotheses and conceptual models in the light of the available BRIE data?

The further revised model provided excellent qualitative reproductions of the observed traces and wetting patterns. The bentonite-wetting model clearly demonstrated the dominant impact of discrete inflow planes on the three-dimensional, non-uniform re-saturation process, which affects wetting times.

Nevertheless, given 1) that the model had to be conditioned to these same traces, 2) that estimating transmissivity and predicting connectivity of the fractures that supply water to the bentonite remained difficult, and 3) that the bentonite itself may play a potentially dominant role somewhat diminishes the presumed power of a DFN for the simulation of deposition holes emplaced in fractured rock.

The observation that the fracture traces generated by the DFN are consistent with the wetting patterns seen on the bentographs – and the related conclusion that most fractures are thus likely to be water-conducting – is most relevant (and partly contradicting the views of other modelling groups).

Water-uptake test

The excellent reproduction of data from the water-uptake test gave confidence into the ability to simulate water imbibition into a homogeneous, partially saturated bentonite block.

Overall

Did the work improve the scientific understanding of the exchange of water across the bentonite-rock interface, and help better predict the wetting of the bentonite buffer? Did the work improve the characterisation methods of the canister boreholes and help establish deposition hole criteria?

The use of a DFN provided considerable insights into the role of the fracture network in supplying water to the bentonite along discrete traces. The work shows the sensitivity of different conceptual and parametric changes in fracture properties on inflow, and specifically highlights the range of prediction results obtained by different DFN realizations. The modelling approach provided simulation results that qualitatively resembled the wetting patterns seen in the bentographs. The focus on discrete flow through a fracture network reproduces the phenomenological behaviour of the interaction between the fractured bedrock and the partially saturated bentonite. The large variability in predicted patterns suggests, however, that predictive modelling remains a challenge even with extensive characterization data, considerable conditioning and calibration: The apparently realistic representation of fractures in a DFN model may not translate into high predictive accuracy. Key concepts – such as connectivity, flow channelling within fracture planes, flow along and across fracture intersections – seem to be difficult to capture even with an extensive, carefully constructed DFN model that focus on measureable geometry. While the sampling bias due to orientation and dimensionality is accounted for, many other assumptions and artefacts remain largely unexplored.

The study highlights the importance that small-scale fractures need to be included to predict bentonite wetting. However, the chosen modelling approach is not fully compatible with the view that small fractures are important, as a) fractures smaller than the mapping cut-off length were not included in the DFN, and b) flow through the rock mass between the larger fractures was ignored, preventing the approximate inclusion of small-fracture effects into the model.

The results from multiple realizations indicated that borehole-specific small-scale characterization of fractures is important if the aim is to predict short-term bentonite behaviour (the study submits a homogenizing effect of bentonite in the long term). This information may be useful when developing deposition hole acceptance criteria.

3.4 Modelling group: KAERI

Section 2.3 summarizes the work and interpretation of KAERI as described in the project report Kim et al. (2018). Technical review comments are documented in the related SKB Review Statement. The following are some remarks that relate the accomplished work to the main objectives. KAERI did not report on Task 8f and did not simulate the water-uptake test.

Task 8A

Did the work identify a suitable method for incorporating bentonite in numerical groundwater flow models, and was the effect of different implementations of the bedrock-bentonite interface evaluated? Did the work provide insights regarding the importance of fractures?

KAERI demonstrated in this initial exercise that their continuum approach and model setup using TOUGH2 yielded results that are consistent with those using similar conceptualizations and assumptions.

Task 8B

Did the work identify a suitable method for incorporating unsaturated, fractured rock and to examine effects of different concepts, boundary conditions, and properties on bentonite re-saturation?

Multiple configurations were tested (intact rock, deterministic geologic structures only, stochastic fracture network only, and combination of deterministic and stochastic fractures) to determine effective properties and to evaluate the relative significance of deterministic and stochastic features. These analyses were insightful, but were done using assumptions that are not easily transferrable to the ultimate geometry and hydrogeology at BRIE. The bentonite re-saturation calculations were then based on a highly idealized homogeneous continuum model. The work is a valid attempt at addressing the objectives of Task 8B; discussion and interpretation of the results was limited; the conclusions thus remained somewhat ambiguous.

Task 8C

Did the work predict inflows and inflow characteristics to deposition holes, and examine the importance of deformation zones and fractures on bentonite re-saturation?

A rather complex sequence of models was used to arrive at predictions of inflow into open holes with different diameter (i.e. into probing holes and collocated surrogate deposition holes). The description of the approach and how it translated into the prediction of bentonite re-saturation was not very transparent. Much of the complexity of the initial models was removed for the final simulation model, which thus lacked the hydrogeologic structures needed to examine the impact of fractures on bentonite re-saturation.

Task 8D

Did the work predict inflows and inflow characteristics to open probing and surrogate deposition holes and examine the impact of fractures and heterogeneity in fractures and matrix on bentonite re-saturation?

While the model was further refined (mainly by including additional monitoring boreholes), the results were considered unreasonable due to a wrong implementation of boundary conditions in these additional holes. The conclusion that additional structural data are needed to accurately predict bentonite re-saturation is partly contradicted by the chosen approach, which eliminates such details in the final step, preventing the model from examining heterogeneous bentonite wetting through discrete features.

Overall

Did the work improve the scientific understanding of the exchange of water across the bentonite-rock interface, and help better predict the wetting of the bentonite buffer? Did the work improve the characterisation methods of the canister boreholes and help establish deposition hole criteria?

KAERI undertook considerable efforts to understand and implement fracture network information into a computationally tractable model capable of simulating bentonite wetting. The use of multiple codes and approaches for generating discrete fractures, continuum meshes, equivalent permeabilities on the scale of computational elements and on the scale of the model domain, and how information is ported from one model to the next is not very transparent. The conclusion that the approach does not yield defensible equivalent permeabilities without an additional calibration step (which was not undertaken) indicates some of its shortcomings. Nevertheless, each model provided insights into the hydraulic behaviour of the considered subsystem. A clear and full documentation of the study is thus desirable.

3.5 Modelling group: LANL

Section 2.4 summarizes the work and interpretation of the LANL modelling group as described in Chapter 3 of the report Dittrich et al. (2014). Technical review comments are documented in the related SKB Review Statement. The following are some remarks that relate the accomplished work to the main objectives. LANL only addressed Task 8D.

Task 8D

Did the work predict inflows and inflow characteristics to open probing and surrogate deposition holes and examine the impact of fractures and heterogeneity in fractures and matrix on bentonite re-saturation?

A new discretization approach was presented that allows for a detailed and accurate representation of complex natural and engineered features. The simulations demonstrate that bentonite wetting is affected by the discreteness of inflow from a connected fracture network. Matrix effects were not considered. The statement that no significant differences in bentonite-wetting results were expected between DFN realizations that were based on the same statistical fracture characteristics may indicate that accurate discretization of the DFN is of reduced significance for the overall purpose of the model. It should also be noted that this statement is contrary to the conclusion reached by the JAEA modelling group.

Overall

Did the work improve the scientific understanding of the exchange of water across the bentonite-rock interface, and help better predict the wetting of the bentonite buffer? Did the work improve the characterisation methods of the canister boreholes and help establish deposition hole criteria?

The new discretization method appears powerful in combining discrete fracture networks with underground structures and volumetric components (such as a bentonite-filled deposition hole). The report focuses on the mesh generation aspects; it does not discuss or interpret simulation results, and no conclusions were drawn beyond the assertion that the new discretization scheme is powerful. In particular, the relative importance of bentonite, deterministic and stochastic fractures, and the background rock was not systematically examined. Such an investigation (along with other sensitivity studies) would have provided valuable perspectives on the need for an accurate representation and discretization of fractures and their connections to the bentonite for the prediction of bentonite wetting.

3.6 Modelling group: NDA-AMEC

Section 2.5 summarizes the Task 8C and 8D work and interpretation of NDA-AMEC as described in the project reports Baxter et al. (2014a, b, 2018a, b). Technical review comments are documented in the related SKB Review Statement. The following are some remarks that relate the accomplished work to the main objectives.

Task 8C

Did the work predict inflows and inflow characteristics to deposition holes, and examine the importance of deformation zones and fractures on bentonite re-saturation?

The simulation approach chosen by AMEC includes the impact of heterogeneity from flow through a discrete fracture network, and at the same time handles the two-phase processes occurring in the bentonite. The considerable influence of heterogeneity as well as the role of the background rock permeability were clearly demonstrated.

Task 8D

Did the work predict inflows and inflow characteristics to open probing and surrogate deposition holes and examine the impact of fractures and heterogeneity in fractures and matrix on bentonite re-saturation?

The study met the objectives of Task 8D by providing detailed results and discussions of inflows into open boreholes and bentonite re-saturation behaviour and times. In particular, different conceptual variants and parameter combinations were examined, providing insights into influential features and properties.

Task 8F

Did the work predict inflows and bentonite wetting characteristics that were consistent with the data collected during the BRIE experiment, including the data obtained after dismantling? Did the work comment on the validity of the initial hypotheses and conceptual models in the light of the available BRIE data?

Further model refinement and partial calibration against available data from the dismantling of BRIE resulted in improved reproduction of the measured data. Comparison with earlier conceptualisations and parameterisations were made, providing insights into the validity of the model. Non-uniqueness and remaining uncertainties and ambiguities were acknowledged. The summaries and discussions in the concluding section are most useful.

Overall

Did the work improve the scientific understanding of the exchange of water across the bentonite-rock interface, and help better predict the wetting of the bentonite buffer? Did the work improve the characterisation methods of the canister boreholes and help establish deposition hole criteria?

AMEC discussed the fact that large variabilities of predicted inflows prevented a formal calibration of a DFN beyond a confirmation that the order-of-magnitude estimates are consistent with observations. Only with this background information may it be considered appropriate to proceed with a single realization. AMEC also recognized the potential sampling bias and the need to account for inflow from the rock mass that includes unmapped and/or un-modelled fractures. These insights were used as the basis for developing an approach that combines DFN and continuum models, which improved scientific understanding of the interaction between the natural and engineered systems. The DFN calibration process proposed by AMEC suggests that considerable characterization data are needed to properly condition the DFN. Examining the relative value of deterministic and stochastic characterization data would be an important research topic that could be addressed by AMEC. Moreover, it would have been very interesting to see an assessment of the ability of the AMEC model to predict bentonite wetting by comparison of modelling results with data collected during bentonite dismantling (as was the objective of Task 8F). In general, the AMEC study is exemplary in its detailed analysis and complete documentation of available characterization data, modelling assumptions, simulation results and their interpretation, which all support insightful conclusions drawn from this modelling exercise.

3.7 Modelling group: Posiva-VTT

Section 2.6 summarizes the work and interpretation of Posiva-VTT as described in the project report Pulkkanen (2018). Technical review comments are documented in the related SKB Review Statement. The following are some remarks that relate the accomplished work to the main objectives.

Task 8A

Did the work identify a suitable method for incorporating bentonite in numerical groundwater flow models, and was the effect of different implementations of the bedrock-bentonite interface evaluated? Did the work provide insights regarding the importance of fractures?

The decision to develop a model that unifies the natural and engineered system components and uses the relevant flow processes (saturated and unsaturated flow) yielded a defensible modelling approach that was further corroborated by obtaining consistent results with two codes that are using very different numerical schemes and discretization methods.

Task 8B

Did the work identify a suitable method for incorporating unsaturated, fractured rock and to examine effects of different concepts, boundary conditions, and properties on bentonite re-saturation?

Unsaturated flow in the bentonite as well as desaturation of the bedrock in the vicinity of the deposition holes as a result of water imbibition into the bentonite was correctly captured using the proposed modelling approach.

Task 8C

Did the work predict inflows and inflow characteristics to deposition holes, and examine the importance of deformation zones and fractures on bentonite re-saturation?

The model and calibration process clearly identified the key characteristics and properties affecting bentonite re-saturation**.**

Task 8D

Did the work predict inflows and inflow characteristics to open probing and surrogate deposition holes and examine the impact of fractures and heterogeneity in fractures and matrix on bentonite re-saturation?

The adjustments made to the model, its calibration, and the study of the impact of mechanical effects on local permeability fields provided a defensible approach to examine bentonite re-saturation and the relative importance of the different elements of the model, specifically that of the background rock, discrete features intersecting the deposition hole, and skin zone properties. The detailed discussion on conceptual and parametric uncertainties concluded that geomechanical effects have a minor impact on the modelled bentonite rewetting.

Task 8F

Did the work predict inflows and bentonite wetting characteristics that were consistent with the data collected during the BRIE experiment, including the data obtained after dismantling? Did the work comment on the validity of the initial hypotheses and conceptual models in the light of the available BRIE data?

Task 8F was used not only to refine certain features, but also to simplify the conceptual model based on insights gained by the comparison between observed and simulated system behaviour. This abstraction process led to a better understanding of the key features and at the same time revealed aspects of the model that were not properly captured. As a whole, Task 8F is a comment on the validity of the initial hypotheses and as such a very good contribution to the overall objectives of Task 8.

Overall

Did the work improve the scientific understanding of the exchange of water across the bentonite-rock interface, and help better predict the wetting of the bentonite buffer? Did the work improve the characterisation methods of the canister boreholes and help establish deposition hole criteria?

The suite of models and simulation studies was systematically developed, with each subtask making use of the conclusions from the previous analyses. The conceptual model is solid, and results support main findings. Modelling results were interpreted and discussed in detail, and conceptual and parametric uncertainties were examined. Key assumptions and alternative conceptual models (specifically that of a discrete fracture network model) were discussed, and the reasons for adopting or rejecting them were given. These discussions are considered most useful and probably one of the main contributions to the overall Task 8 project. The studies increased the understanding of the relative importance of the natural and engineered system components, which can be used to develop more effective characterization methods and deposition hole siting criteria.

3.8 Modelling group: SKB-CFE-Golder

Section 2.7 summarizes the work and interpretation of the SKB-CFE-Golder team. Technical review comments are documented in the related SKB Review Statement. The following are some remarks that relate the accomplished work to the main objectives.

Task 8A

Did the work identify a suitable method for incorporating bentonite in numerical groundwater flow models, and was the effect of different implementations of the bedrock-bentonite interface evaluated? Did the work provide insights regarding the importance of fractures?

It was demonstrated that bedrock, fractures, and bentonite could be simulated using a single model. However, partially saturated conditions were only accounted for in the bentonite, whereas only saturated conditions were considered in the natural system. The impact of this simplifying assumption was not examined, even though DarcyTools can handle partially saturated conditions in the entire model domain. A comparison between these two approaches would be very useful to assess the error made by ignoring unsaturated flow effects in the bedrock.

Task 8C

Did the work predict inflows and inflow characteristics to deposition holes, and examine the importance of deformation zones and fractures on bentonite re-saturation?

Inflow characteristics were visualized, showing the importance of the distribution of discrete inflow points to the re-saturation pattern and wetting time. Sensitivity analyses were performed with respect to stochastic fracture network parameters. In addition, multiple realizations were evaluated. The resulting variability in predicted inflow was substantial in that inflow is relatively small, but less relevant for Borehole KO0014G01, which had the largest average inflow. If a large geologic structure was relocated to intersect the boreholes, it had the expected dominant effect. Finally, the simulations indicated that partially saturated conditions would develop in the fractured rock around the bentonite-filled deposition holes; this effect was not accounted for in the Task 8C modelling.

Task 8D

Did the work predict inflows and inflow characteristics to open probing and surrogate deposition holes and examine the impact of fractures and heterogeneity in fractures and matrix on bentonite re-saturation?

The simulations examined inflow patterns, the impact of widening the probing holes to create surrogate deposition holes, and variability and uncertainty due to the stochastic nature of the fracture network. Unfortunately, the time discretization effects and erratic inflows from open boreholes were not resolved. While partially saturated conditions in the bedrock were considered in the Task 8D simulations, no systematic analysis of this effect was undertaken.

Overall

Did the work improve the scientific understanding of the exchange of water across the bentonite-rock interface, and help better predict the wetting of the bentonite buffer? Did the work improve the characterisation methods of the canister boreholes and help establish deposition hole criteria?

The conceptual model (specifically that used in Task 8D) accounts for the coupling of the engineered and natural systems, and includes the effects of large geologic structures, stochastic fracture networks, and the background rock on inflow and bentonite wetting. The number, location, and transmissivity of individual fractures intersecting the deposition holes affected bentonite re-saturation patterns and thus wetting times. Considerable differences between stochastic realisations were observed, leading to the conclusion that the models should be conditioned to fracture information observed at a site and in individual deposition holes. The simulations appear significantly influenced by the chosen time discretisation. While a powerful tool was applied to the study of fracture-matrix interaction effects, questions remain about its accuracy at the bentonite-rock interface. Moreover, no attempts were made to condition the fracture network or to calibrate the model, and only limited sensitivity analyses were performed.

3.9 Modelling group: SKB-Clay Technology

Section 2.8 summarizes the modelling work and interpretation of SKB-Clay Technology as described in the project report Malmberg and Åkesson (2018). Technical review comments are documented in the related SKB Review Statement. The following are some remarks that relate the accomplished work to the main objectives.

Task 8A

Did the work identify a suitable method for incorporating bentonite in numerical groundwater flow models, and was the effect of different implementations of the bedrock-bentonite interface evaluated? Did the work provide insights regarding the importance of fractures?

The objectives of Task 8A were met by demonstrating the use of the software Code_Bright for the simulation of both the bedrock and bentonite. Moreover, the investigated sensitivity cases provided some insights into the relative importance of matrix, fracture, and bentonite parameters.

Task 8C

Did the work predict inflows and inflow characteristics to deposition holes, and examine the importance of deformation zones and fractures on bentonite re-saturation?

Inflow measurements were used to calibrate the model. The effect of a single (observed) fracture intersecting the deposition hole on bentonite re-saturation was demonstrated, and the effect of an impermeable plate at the bottom of the borehole was examined.

Task 8D/F

Did the work predict inflows and bentonite wetting characteristics that were consistent with the data collected during the BRIE experiment, including the data obtained after dismantling? Did the work comment on the validity of the initial hypotheses and conceptual models in the light of the available BRIE data?

The model reproduced the observed inflows reasonably well and predicted relative humidity in the bentonite with acceptable deviations. The impact of discrete inflows from fractures on bentonite re-saturation became evident with the sensitivity of the position of the relative humidity (RH) sensor with respect to the fracture location. The RH data also provided conclusive evidence about the low background rock permeability.

Water-uptake test

Additional confidence into the proposed modelling approach was gained by simulating the water-uptake test and comparing the calculated saturation, relative humidity, and cumulative imbibition to the measured data.

Overall

Did the work improve the scientific understanding of the exchange of water across the bentonite-rock interface, and help better predict the wetting of the bentonite buffer? Did the work improve the characterisation methods of the canister boreholes and help establish deposition hole criteria?

The simulation studies, model calibration, sensitivity analyses, and comparisons between predicted and measured data were well interpreted. The report also contained sub-analyses undertaken to examine assumptions and the validity of certain decisions and approaches (e.g. analysis of initial gap between bentonite and deposition hole wall; evaluation of relative permeabilities derived from vapour permeability data; scale-dependence of hydraulic conductivity). These analyses – along with detailed descriptions of assumptions and interpretations of data and modelling results – made this study transparent and defensible. It thus considerably improved the scientific understanding of key features and processes determining bentonite re-saturation in a fractured bedrock. Clay Technology has been directly involved in the experimental aspects of BRIE and WUT, giving them additional information and insights.

3.10 Modelling group: SKB-KTH

Section 2.9 summarizes the work and interpretation of Royal Institute of Technology (KTH), Stockholm, Sweden. Technical review comments are documented in the related SKB Review Statement. The following are some remarks that relate the accomplished work to the main objectives.

Task 8A

Did the work identify a suitable method for incorporating bentonite in numerical groundwater flow models, and was the effect of different implementations of the bedrock-bentonite interface evaluated? Did the work provide insights regarding the importance of fractures?

Task 8A demonstrated that the proposed method was capable of simulating water flow under both saturated and partially saturated conditions in a porous medium that may contain a discrete feature. It showed the expected influence of the fracture on the pressure distribution.

Overall

Did the work improve the scientific understanding of the exchange of water across the bentonite-rock interface, and help better predict the wetting of the bentonite buffer? Did the work improve the characterisation methods of the canister boreholes and help establish deposition hole criteria?

The work can be considered a code verification exercise using Task 8A as a test case. No scientific or technical questions were addressed. The early-time discrepancies between simulations that use two different fracture representations were noted, but not explained. No conclusions were derived from the study.

3.11 Modelling group: SKB-Stockholm university

Section 2.10 summarizes the work and interpretation of Stockholm University as described in the project report Dessirier et al. (2017). Technical review comments are documented in the related SKB Review Statement. The following are some remarks that relate the accomplished work to the main objectives.

Task 8A

Did the work identify a suitable method for incorporating bentonite in numerical groundwater flow models, and was the effect of different implementations of the bedrock-bentonite interface evaluated? Did the work provide insights regarding the importance of fractures?

Rock-bentonite interaction is simulated in a single, fully coupled model that accounts for two-phase flow, gas dissolution, and trapping mechanisms and the desaturation of the rock. Different scenario evaluations indicated that neglecting the presence of the gas phase leads to systematic under-prediction of bentonite wetting times. The impact of fracture positions was also evaluated. The study thus addressed the task objectives and provided additional insights into two-phase processes and the potential errors made by neglecting them.

Task 8B

Did the work identify a suitable method for incorporating unsaturated, fractured rock and to examine effects of different concepts, boundary conditions, and properties on bentonite re-saturation?

A relatively complete representation of two-phase flow phenomena in a model that includes both the fracture rock and the bentonite was used to examine bentonite re-saturation in the presence of air.

Task 8C

Did the work predict inflows and inflow characteristics to deposition holes, and examine the importance of deformation zones and fractures on bentonite re-saturation?

Predicted inflows were used as calibration targets of the model.

Task 8D

Did the work predict inflows and inflow characteristics to open probing and surrogate deposition holes and examine the impact of fractures and heterogeneity in fractures and matrix on bentonite re-saturation?

The presence, location, and hydrogeologic properties of fractures were examined in a scenario analyses.

Task 8F

Did the work predict inflows and bentonite wetting characteristics that were consistent with the data collected during the BRIE experiment, including the data obtained after dismantling? Did the work comment on the validity of the initial hypotheses and conceptual models in the light of the available BRIE data?

Simulation results were compared to measured data. An approach was developed to better include bentonite dismantling data in the analysis. The comparison between model results and observations was consistently used to examine the validity of modelling assumptions, specifically those related to the impact of the gas initially present in the bentonite on re-saturation time.

Overall

Did the work improve the scientific understanding of the exchange of water across the bentonite-rock interface, and help better predict the wetting of the bentonite buffer? Did the work improve the characterisation methods of the canister boreholes and help establish deposition hole criteria?

The focus of the SKB-SU modelling was on evaluating two-phase flow dynamics and their impact on saturation distributions and re-wetting times. As such, the modelling provided scientific insights into the appropriateness and potential bias introduced by using simplifying modelling assumptions (such as fully saturated flow conditions or the use of Richards' equation). The fate of air initially present in the bentonite as examined in these modelling studies is of potential significance as it affects biogeochemical reactions and corrosion rates. In addition, the modelling group developed a method to improve the quantitative analysis of grey-scale bentograph pictures and corresponding water content measurements, which is essential for a correct interpretation of the processes occurring at and across the interface. All these analyses, while not strictly following the objectives of the task description, yielded results and insights that are relevant to the topic examined by Task 8.

3.12 Modelling group: Technical university of Liberec

Section 2.11 summarizes the work and interpretation of Technical University of Liberec as described in the project report Hančilová and Hokr (2018). Technical review comments are documented in the related SKB Review Statement. The following are some remarks that relate the accomplished work to the main objectives.

Task 8A

Did the work identify a suitable method for incorporating bentonite in numerical groundwater flow models, and was the effect of different implementations of the bedrock-bentonite interface evaluated? Did the work provide insights regarding the importance of fractures?

While the use of a diffusion equation with nonlinear diffusivities is a valid approach to simulate systems based on the Richards equation, the fact that the material properties needed to be adjusted significantly to reproduce the reference solution provided in Vidstrand et al. (2017) indicates either that different cases were simulated, or that the implementation of the diffusion equation is flawed. The derived conclusions regarding the relative impact of fracture, background rock, and bentonite properties thus need to be reassessed.

Task 8D

Did the work predict inflows and inflow characteristics to open probing and surrogate deposition holes and examine the impact of fractures and heterogeneity in fractures and matrix on bentonite re-saturation?

The simulations demonstrated the general characteristics of bentonite re-saturation (timing and patterns) and the impact of individual fractures and the background rock using a simplified representation of the interface between the bentonite and the formation.

Overall

Did the work improve the scientific understanding of the exchange of water across the bentonite-rock interface, and help better predict the wetting of the bentonite buffer? Did the work improve the characterisation methods of the canister boreholes and help establish deposition hole criteria?

The modelling team demonstrated that unsaturated flow and bentonite rewetting could be simulated using a diffusion equation with non-constant hydraulic diffusivities. However, the implementation of this approach needs to be further verified before reliable predictions can be made. Moreover, the model used for simulating bentonite wetting is not fully coupled to a model of the bedrock. Nevertheless, general insights into the saturation patterns and wetting times were obtained. No scientific conclusions were drawn from the study.

4 Preliminary comparative analysis

4.1 Introduction

The modelling groups participating in the SKB Task Force (see Table 1-1) not only worked on the understanding and modelling of the various subtasks related to Task 8, but also exchanged information and discussed modelling issues at 10 Task Force meetings and numerous workshops. Moreover, the integration of experimental work (BRIE and WUT) and active participation of the experimenters in the Task Force meetings further helped focus the research to address common topics and issues. While these interactions are considered fruitful and beneficial to each group's research goals, the modelling results were generally presented as the outcome of relatively independent, stand-alone research work.

The fact that 11 modelling groups addressed a common set of questions using disparate data interpretations, conceptualizations, modelling approaches and simulation codes provided a unique opportunity for a comparative analysis. While a comparative analysis was not called out as an explicit goal of this Task 8, the potential benefits of looking at the ensemble of results, conclusions, and recommendations was recognized by the participants, who provided additional information and detailed descriptions of their modelling approach (see Section 1.7 and Appendix A) in support of such an analysis.

The purpose of the preliminary comparative analysis presented in this section is not to identify the "correct" predictive value of, for example, the bentonite re-saturation time; instead, the goal is to obtain some insights into the variability in predictive results, which has to be expected given uncertainties in data, conceptualizations, parameter values, and simulation approaches. This insight can best be gained by stepping outside the specific framework chosen by each modelling group. More importantly, the various interpretations of data and simulation results, and the evaluation of all findings improve overall system understanding and are likely to help identify areas where the knowledge can be considered sufficient or where further research is needed.

The purpose of this section is to present some of the similarities and differences in assumptions and results, and to compile the quantitative performance measures calculated by most of the modelling groups. They are related to the key elements, processes, and modelling issues summarized in Figure 1-1. A comparison of performance measures and interpretation of conceptual model uncertainties is largely outside the scope of this evaluation report, but is partly addressed in Finsterle et al. (2018).

This section (as well as Chapter 5) contains some evaluative comments that refer to the Task 8 as a whole. The comments are thus summary statements that may not properly reflect the work of individual modelling groups (which was commented on in Chapter 3).

4.2 Software tools

4.2.1 Codes used

Task 8A aimed at identifying a modelling approach and associated software suitable for simulating groundwater flow from fractured rock across an interface into initially partially saturated bentonite (Section 1.5.3). While not designed as a code comparison study, each modelling group simulated a well-defined test case (Task 8A) using a variety of software tools (Table 4-1). The software tools ranged from well-established reservoir simulators to general-purpose PDE solvers to adaptations of existing tools for the incorporation of partially saturated conditions to new developments based on alternative formulations of the governing equations. The codes numerically solved either the Richards equation, a two-phase formulation of Darcy's law, the hydraulic diffusion equation with non-constant diffusion coefficients, or the saturated flow equation with the storativity term adjusted to mimic partially saturated conditions. While the simulation of fully coupled thermal-hydrogeological-mechanical-chemical processes was outside the scope of Task 8, some modelling groups examined coupled hydrogeological-mechanical effects on property and inflow distribution.

In some cases, multiple tools were used, each dedicated to solving the flow problem particular to one of the two subsystems (fractured rock and bentonite). They were used without coupling, with one-way coupling, or iterative coupling. Most modelling groups used a single tool to simulate both subsystems in an integrated manner.

Table 4-1. Software tools used by modelling groups.

Modelling Group	Software	Comments, Reference
GRS	d^3f VIPER	Bedrock (Schneider 2012) Bentonite (Kröhn 2011, Kröhn 2017, App. F)
JAEA	FracMan MAFIC Thames MTOT, TTOM	Bedrock (Dershowitz et al. 2007) Bedrock (Miller et al. 2001) Bentonite THM (Chijimatsu et al. 2000) Interface utility programs
KAERI	TOUGH2 FracMan/MAFIC FLAC3D COMSOL	Bedrock and bentonite (Pruess et al. 1999) Determination of effective permeabilities Steady-state saturated flow Mesh generation
LANL	LaGriT FEHM	Mesh generation (LaGriT 2011) Two-phase flow (Zyvoloski 2007)
NDA-AMEC	ConnectFlow TOUGH2	Saturated DFN flow (AMEC 2012) Two-phase flow (Pruess et al. 1999)
Posiva-VTT	COMSOL TOUGH2	COMSOL Multiphysics. 2008b. COMSOL Multiphysics Modeling Guide: Version 3.5 Stockholm, Sweden: COMSOL AB. COMSOL Multiphysics. 2008b. COMSOL Multiphysics Modeling Guide: Version 3.5 Stockholm, Sweden: COMSOL AB. COMSOL Multiphysics. 2008b. COMSOL Multiphysics Modeling Guide: Version 3.5 Stockholm, Sweden: COMSOL AB COMSOL Multiphysics. 2008b. COMSOL Multiphysics Modeling Guide: Version 3.5 Stockholm, Sweden: COMSOL AB All simulations (http://www.comsol.com/) Benchmarking (Pruess et al. 1999)
SKB-CFE-Golder	DarcyTools	(Svensson et al. 2011)
SKB-Clay Tech	Code_Bright COMSOL	(Olivella et al. 1996) (http://www.comsol.com/)
SKB-KTH	Own development	Pressure formulation for saturated and unsaturated flow in fractured system
SKB-SU	TOUGH2	Richards' equation and two-phase flow formulation (Pruess et al. 1999)
TUL	Ansys Flow123D	ANSYS (2010)

4.2.2 Comments on software tools

Based on the results of Task 8A, most of the software tools selected, adapted, or developed by the modelling groups are likely to be suitable for simulating flow through fractured rock and hydration of bentonite. This statement must be qualified by noting that the reference solution for Task 8A is also a simulation result rather than an interpretation of observations from a real system. Given that the reference solution itself is subject to simplifications and assumptions, agreement with that solution only confirms that the various codes solve the same or similar sets of equations in a consistent manner; it does not confirm, however, that a model using a specific code captures the actual system behaviour appropriately.

It appears that the choice of a simulator was mainly guided by code availability and the modelling group's familiarity with the software. Code capabilities then drove the conceptual model development.

A more defensible approach would be to first analyse the features, events, and processes that are considered relevant for the system to be simulated, and by considering the objectives of the study. Only after the conceptual model is developed and the required simulation capabilities are identified should the software tools be selected.

The range of outcomes simulated with the chosen simulation tools is limited by the codes' capabilities, which may be significantly smaller than the range of the system behaviour itself. This is relevant, as such a limitation potentially yields a non-conservative prediction of repository performance.

The limitations of the codes (specifically regarding implemented features and processes) and how they impacted the conceptual model chosen for the Task 8 analyses should be discussed in detail. Moreover, alternative conceptualisations – even if they were not examined by numerical simulation – should be described.

4.2.3 Comments on subsystem coupling

As mentioned in Section 4.2.1, some modelling groups used separate codes to simulate the natural and engineered barrier systems. Different coupling strategies were employed:

- *No direct coupling*:

  Information about the system state in the rock was transferred to the simulation of bentonite hydration in only a qualitative or conceptual manner.

- *One-way coupling*:

  Information about the system state in the rock was transferred to the simulation of bentonite hydration in a quantitative manner (e.g. by specifying flow rates at the bentonite surface), but without accounting for feedback mechanisms between the two subsystems.

- *Iterative coupling*:

  State variables from one subsystem were specified as boundary conditions for the other subsystem; they were iteratively updated.

The approach of separating processes and subsystems and studying them separately has the following advantages:

- It enables the use of specialized modules for each of the subsystems. For example, a discrete fracture network model can be developed to represent saturated flow in the fractured rock, and a continuum model can be developed to simulate two-phase flow in the bentonite.
- The strategy used to link the two models may provide an opportunity to implement or otherwise account for specific, difficult-to-simulate processes occurring at the interface between the two subsystems.
- The need to conceptually separate the two subsystems may help identify key features and flow regimes (e.g. the recognition that bentonite hydration is either limited by water supply from the fractured rock, or by the capacity of the bentonite to absorb the water, which is provided in abundance from the rock).
- The approach may be computationally more efficient because a) the system of fully coupled partial differential equations is smaller, and b) only the processes relevant for each subsystem need to be captured (e.g. two-phase flow conditions only need to be simulated in the bentonite, whereas fully saturated conditions can be assumed in the fractured rock).

The approach may have the following limitations:

- Treating the subsystems separately requires the development of a linking strategy between the two codes and models. This likely induces additional modelling errors that are difficult to detect or quantify. Moreover, it may make the approach less transparent.
- Unless an iterative coupling scheme is employed, the approach may not be able to account for feedback mechanisms between the two subsystems.

The second, "one-model-fits-all" approach, in which both the natural and engineered barrier systems are simulated using a single code and model, has the following advantages:

- A fully integrated treatment of the entire system may be considered more transparent.
- The approach automatically accounts for feedback mechanisms between the two subsystems.

The approach may have the following limitations:

- A single model may not be able to optimally represent the specific processes in each of the subsystems. Moreover, processes at the interface between the two systems, which may be fundamentally different, cannot readily be included.
- Simultaneously solving all governing equations of the entire system is computationally demanding.

Each modelling group chose an approach ("divide-and-conquer" vs. "one-model-fits-all") that seemed appropriate for their conceptual model, available software, and research focus. Unfortunately, with a few exceptions, it is not evident that special consideration was given to the processes occurring at or across the interface between the bentonite and fractured rock. Given that understanding the interaction between the two subsystems across this interface was a prominent topic of Task 8, a detailed discussion of the interface would have been most useful. Both approaches provided opportunities to examine these processes, either by implementing them into the coupling strategy or by explicitly including an interface zone in the integrated numerical model.

4.3 Comparison of modelled processes

The modelling groups made decisions about the processes that needed to be simulated. The task description and specifically the objectives of Task 8A indicated that the main processes to be considered included fluid flow through fractured rock and imbibition into partially saturated bentonite. It was recognized that mechanical effects may be important for both the natural and engineered barrier systems, as damage from the drill-and-blast excavation of the TASO tunnel and the stress changes induced by the open tunnels and boreholes may affect the characteristics of the fractures intersecting the openings (which are the most influential features for bentonite wetting), and the swelling pressure of the bentonite may change its inherent hydraulic properties. While simulating coupled hydrogeological-geomechanical processes was not considered a priority in Task 8, one modelling group studied stress redistribution near the deposition hole and its impact on local fracture transmissivities, and another evaluated bentonite swelling and the related closing of the interface gap. To limit the complexity and scope of Task 8, it was also decided to ignore thermal and geochemical processes despite their likely impact on the system behaviour. (Note that BRIE was designed was designed as an isothermal experiment partly to minimize such complicating coupled effects.) Some modelling groups included the expected effects of coupled processes on near-borehole conditions by specifying skin zones. Density effects (due to salinity) were discussed, but not implemented in any of the models.

Flow processes were represented using one of the following governing equations:

- *Saturated flow using Darcy's law*:

  Darcy's law was used to simulate flow through porous media for both the fractures and (if included in the model) the rock mass in between fractures. The underlying assumption of fully liquid saturated conditions ignores the potential desaturation of the formation near the bentonite-rock interface. A separate model is used to simulate the partially saturated bentonite (see Section 4.2.3).

- *Simplified saturation method (SIMSAT):*

  One modelling group developed a method referred to as simplified saturation method (SIMSAT), in which the storativity term in the balance equations for saturated flow is modified to account for the increase in water storage volume available under partially saturated conditions.

- *Diffusion equations:*

  Unsaturated flow was modelled using a diffusion equation with a nonlinear, saturation-dependent diffusion coefficient. One group developed a model that accounted for diffusive flow of vapour in the pore space as well as that of interlamellar water.

- *Richards' equation:*

  Flow of water under partially saturated conditions was modelled using Richards' equation, which accounts for relative permeability and capillary pressure effects of the liquid phase, but ignores the presence of a viscous, compressible, and dissolvable gas phase.

- *Two-phase flow formulation:*

  A two-component (water and air), two-phase (liquid and gas) formulation accounts for flow and potential trapping of the gas initially present in the bentonite.

The different approaches to simulate the flow conditions in the bentonite and fractured rock all appear valid approximations. A detailed discussion of the underlying assumptions and their potential impact on the simulation results and conclusions is desirable. It is also noted that some parameter adjustments were needed in some of the models during the verification exercise of Task 8A, suggesting that the chosen approach is either oversimplified or not properly implemented in the numerical code.

The choice of the governing equations appeared to have an impact on a) the research topic chosen for analysis, and b) the simulation results and conclusions. In particular, using a full two-phase formulation allowed for an analysis of gas trapping, which appeared relevant when calculating the wetting times needed for (almost) complete saturation of the bentonite. Conversely, the impact of potential desaturation of the geosphere could not be analysed when using a saturated flow model. Darcy's law with static and non-hysteretic relative permeability and capillary pressure functions was considered applicable to simulate fluid flow in swelling clays, fractures, fracture zones, and tight background rock. Again, a discussion of this assumption and the potential limits of its applicability would be desirable.

4.4 Comparison of modelling approaches for natural barrier system

In addition to selecting the governing equations that describe the key processes (see Section 4.3), the conceptual model also includes a simplified representation of the system's key hydrogeological and engineered features. This subsection summarises the alternative ways the Task 8 modelling teams represented the geosphere.

It was universally recognized that fractures on various scales are likely to dominate groundwater flow in the geosphere, inflow into open deposition holes, and bentonite wetting. How to appropriately represent individual fractures or the fracture network as a whole was thus a critical conceptual modelling decision.

The task description (Vidstrand et al. 2017) devoted considerable space to the description of the geometry of underground openings (tunnels and boreholes) and the known, large hydrogeological structures identified in the BRIE area. These structures were likely to be implemented as deterministic structures. Smaller-scale fractures were described by means of stochastic parameters. Fracture trace maps were made available, showing the intersection of fractures with tunnels and deposition holes. After dismantling of BRIE, the so-called bentographs provided an additional, detailed view of discrete, water-conducting features for two of the deposition holes.

The modelling groups approached the problem of how to include the effect of a large number of fractures into the numerical model in different ways, arriving at different alternative conceptual models, which in turn led to different emphases of the modelling studies and – more importantly – different conclusions. The approaches used included:

- *Homogeneous, effective continuum model:*

  Continuum models with effective parameters were used by some modelling groups to demonstrate that such an approach would oversimplify the complexity of the system and lead to unreasonable results.

- *Classic discrete fracture network model:*

  Discrete fracture network (DFN) models were used by multiple modelling groups, albeit in different ways and for different purposes. The direct translation of the stochastic information of fracture networks from the task description yielded classic DFN models, whereby multiple realisations of fracture networks that honour these statistics were generated. Some modelling groups conditioned the networks on fracture trace maps, and/or changed the statistics to account for the assumptions that not all fractures conduct water. This approach neglected interaction with the rock mass that is in between the fractures. It also neglects the impact of fractures that were smaller than the cut-off value of the fracture trace length used in tunnel mapping. While certain modelling groups chose to only include a subset of mapped fractures into the model to account for hydraulically inactive fractures, others refer to the bentographs as supporting their view that all mapped fractures are water-conducting and should thus be represented in the model. Finally, these classic DFN simulations handled only fully saturated flow.

- *Discrete fracture network model as basis for a stochastic continuum model:*
  Multiple modelling groups generated DFNs that were then mapped onto a continuum grid. Effective continuum properties were determined (either based solely on geometry or by performing flow simulations) and assigned to each computational grid block, arriving at a heterogeneous continuum model. Different approaches were used to upscale and map fracture properties to the continuum scale. Grid blocks that were not intersected by a fracture were assigned background rock properties.
- *Hybrid discrete fracture network model and continuum model:*
  Some modelling groups posited that the discrete inflows across the rock-bentonite interface critically determine bentonite wetting, whereas the details of the far-field fracture network are insignificant as long as the network provides connectivity from a sufficiently large water source to the near field of the experiment. Based on this conceptualization, they developed a hybrid model in which the mapped fractures intersecting the deposition holes are deterministically implemented into the model, while the far field is presented as a homogeneous, effective continuum.
- *Artificial fractures and skin zones:*
  The large impact of the fractures intersecting the deposition holes prompted the ad hoc inclusion of "artificial fractures" during early development stages of the model. Similarly, skin zones were introduced to account for potential changes in fracture and background rock properties near underground openings.

The list above demonstrates the variety of models developed for the natural barrier system available within the Task 8, which provides a unique opportunity to study the impact of alternative conceptualizations on predictions and conclusions. The wide variety is noteworthy specifically since all models were based on the same, rather extensive set of fracture data provided by Vidstrand et al. (2017) in the task description.

The modelling groups' conceptualisations appear partly driven by their choice of simulation software, specifically the ability to generate stochastic fracture networks. Once this choice was made, however, the subsequent analyses were partly limited (e.g. to saturated flow without consideration of matrix or unmapped small fractures). This may have led to a bias in the conclusions. Conversely, DFN models were able to examine the spread of predictions as a result of spatial variability, randomness, and uncertainty in fracture characterisation.

The modelling groups that developed a hybrid approach generally went through a detailed examination of conceptual issues based on available data and their system understanding. They assessed the potential influence of each natural feature and related modelling component, and discussed the appropriateness of the simplifications they made (specifically the decision not to use a DFN in the far field). This deliberate consideration of the balance between fidelity and computational efficiency generally led to well-documented, defensible conceptual models.

4.5 Comparison of modelling approaches for engineered barrier system

This subsection summarises the alternative ways the modelling groups represented the bentonite. It is generally recognized that bentonite is a special, complex material, mainly because of its swelling capacity, which changes 1) the geometry of the pore space, 2) the way water is adsorbed and transported within the bentonite (both on the pore scale and continuum scale), and thus 3) the hydrogeologic properties that need to be assigned to bentonite in a numerical model (Wieczorek et al. 2017). Moreover, bentonite may readily erode, or the increasing swelling pressure may cause coupled mechanical effects and expulse bentonite into fractures. The swelling properties of bentonite and specifically the relation between saturation, swelling pressure, absolute and relative permeabilities, and capillarity, are complex, non-linear functions that are difficult to measure experimentally and to implement into a numerical model. Impacts of ionic strength and temperature may also need to be accounted for.

Despite this complexity, all modelling groups treated the bentonite as a conventional porous medium. While the parameterisation of the bentonite-wetting model was questioned by one modelling group, the use of classic flow equations and standard relative permeability and capillary pressure functions was considered appropriate for predicting bentonite hydration. This confidence is mainly based on previous modelling of water-uptake in bentonite (both in laboratory and field-scale experiments; Alonso et al. 1998, Gens et al. 2002, Vaunat and Gens 2005) and the success most modelling groups had in reproducing the data from the water-uptake test (WUT). The WUT was a well-controlled laboratory experiment; the measured cumulative water-uptake as well as saturation and relative humidity profiles were well matched by the models with minor adjustments of parameters.

Matching the data from sensors installed in the field and additional information obtained after dismantling of BRIE proved more challenging. Deviations between measured and calculated saturations and relative humidities were mainly attributed to inaccuracies in the relative positioning of sensors and fractures, uncertainty in fracture and background rock inflow rates, and experimental incidents, specifically the accidental flooding of the central tube and intentional filling of the gap between the bentonite and the rock (see Section 4.7 for further comments on the treatment of these incidents).

The confidence in the bentonite model helped reduce ambiguities when analysing data from BRIE dismantling and the associated bentographs. Key uncertainties in model predictions were almost exclusively attributed to uncertainties in the geometry and hydrogeological properties of the fractured rock.

The comparatively high confidence the modelling groups had in their representation of the bentonite appears appropriate. However, the modelling reports could be strengthened by adding a more detailed discussion of the underlying assumptions and the (potentially limited) applicability range of the chosen bentonite model and its parameterisation.

4.6 Representation of bentonite-rock interface zone

The title of Task 8 indicates that special attention is to be given to the interaction between the natural and engineered barrier systems, which occurs at the interface between the fractured rock and the bentonite in a deposition hole. (Note that the term "interface" may be viewed as an interface zone, i.e. it includes part of the bentonite and fractured rock in the immediate vicinity of the contact area between the two materials). It is thus essential to have a good understanding of this interface, specifically its geometry, properties, and the processes by which fluid is exchanged between the two adjacent subsystems. How this interface is represented in the numerical models is likely to affect the evolution of the conditions in both the fractured rock and the bentonite, and it determines the nature, strength, and significance of feedback mechanisms between the two subsystems.

As described in Section 4.2.3, most modelling groups simulated both the natural and engineered barrier systems in a single model, or they developed a (one-way or two-way) coupling strategy that allows the two subsystems to interact with each other. However, none of the modelling groups represented or modelled the interface between the fractured rock and the bentonite as an explicit feature with its own properties or processes. The interface was largely described as an initial gap between the bentonite surface and deposition hole wall after bentonite installation; then the assumption was made that the filling of the gap with water leads to fast and sufficient clay swelling so that no special treatment of the interface is needed.

While neglecting the interface as a feature that requires special attention may be appropriate, no modelling-based justification can be provided, as the interface is not explicitly represented in the models. The modelling approach chosen to link the natural and engineered barrier systems thus remains *ad hoc*, specifically since only limited discussions of the interface were provided in the modelling reports. The bentographs obtained after BRIE dismantling may indicate that the processes occurring at the interface are complex and worthy of special consideration. An incomplete list of potentially influential features and processes at and across the interface is given here as a suggestion of future research topics:

- Development of preferentially vertical features as a result of bentonite installation.
- Potential impact of change of pore size distribution after initially free-swelling bentonite contacts wall of deposition hole.
- Potential impact of change in pore structure and misalignment of fracture apertures and bentonite pores across interface.
- Potential impact of bentonite expulsion into fractures and/or bentonite erosion at contact with fractured rock.
- Potential impact of locally incomplete closure of initial gap, breaking capillary continuity, providing zones for gas accumulations, or creating fast-flow pathways.
- Potential impact of various skin zone effects on both sides of the interface.
- Unsaturated flow effects (bridging, channelization, change in meniscus curvature, film flow, etc.) similar to those seen across fracture intersections (but different from those within fracture planes and/or porous media).
- Potential impact of geomechanical and bentonite-swelling effects.
- Potential impact of change from predominantly linear to radial or spherical flow regime, and change in permeability anisotropy magnitude and orientation.
- Potential impact of very high contrast in fluid flow properties (permeability, wettability, capillarity, porosity, etc.) and transition from single-phase to two-phase conditions across the interface.
- Potential impact of very large initial gradient in water potential across interface.
- Potential effects of natural water inflow into or intentional filling of gap between bentonite and rock on water distribution and imbibition into the bentonite.

4.7 Conditioning and calibration

Task 8 was predominantly devised as a numerical modelling exercise with the goal to improve system understanding. However, the simulations were expected to be done for site-specific conditions, with special consideration of the BRIE layout and testing activities. Tying the modelling to a specific site with the opportunity to compare simulation results to actual field data made Task 8 (as well as some of the previous SKB Task Force projects) more interesting and more relevant, but also more challenging.

The task description provided a considerable amount of characterisation data. Moreover, some of these data had already been analysed and converted to parameter values that could be used directly as input to the numerical models. Implicit in these analyses and parameters were conceptual decisions as well as assumptions and limitations. Most modelling groups adhered to the framework presented in the task description, at least for the initial stages of the study.

Throughout the course of Task 8, experimental data from BRIE were made available to the modelling groups, usually concurrently or ahead of the corresponding simulations. Because of the relative timing of experiments and modelling, no truly blind predictions were made. Yet, the BRIE experiment provided characterisation data that could be used for adjusting conceptual models and calibrating its parameters. The structure of the subtasks (see Section 1.5.2) reflected this workflow, whereby the model was continuously refined as new data became available.

The following information and data were used for conditioning and calibrating the models:

- An analytical or numerical reference solution (for Task 8A).
- High-level description of structural geology and hydrostratigraphy.
- Fracture trace maps at tunnels and deposition holes.
- Fracture statistics.
- Hydraulic properties (including two-phase properties) from core samples.
- Hydraulic properties from in situ flow tests.
- Borehole logs and Borehole Image Processing System (BIPS) data.
- Inflows to tunnels.
- Inflows to open boreholes.
- Pressures in packed-off borehole intervals.
- Pressure and relative humidity data in bentonite.
- Water content, saturation and (bulk and dry) density data from bentonite samples after dismantling of BRIE.
- Cumulative water-uptake and relative humidity profiles from water-uptake test.
- Bentographs after dismantling of BRIE.

Most modelling groups used this information to develop and adjust the conceptual model and to determine select parameters. The features and parameters adjusted by the modelling groups included the following:

- Effective permeability of fractured formation or rock mass between discrete fractures.
- Skin zone permeability.
- Transmissivity of large discrete geologic structures and discrete medium-scale fractures.
- Location and orientation of fractures intersecting the deposition holes.
- Predictive power of probing hole geometry data and interpretation relative to the corresponding geometry deduced from surrogate deposition holes.
- Selection of stochastic DFN realisation.

Most modelling groups evaluated the misfit between model output and measured data either visually or by comparing individual residuals; no formal inversion approach was used. The conditioning and calibration was thus essentially a sensitivity analysis with the measured data as the desirable outcome. The quality of the calibration was judged based on a the residuals; other metrics (such as estimation uncertainty, parameter correlations, or model identification criteria) were not formally evaluated. Nevertheless, some modelling groups commented on the results of the sensitivity analyses and concluded that the calibrations are likely ill-posed, leading to non-unique parameter estimates.

The calibration process had the following notable outcomes:

- The accurate reproduction of the water-uptake test data – with little need for parameter adjustments – gave considerable confidence in the way the bentonite was represented and parameterised in the model (see Section 4.5).
- As parameters are related to the chosen conceptual model, adjusting them to match the observed data necessarily led to a changed perspective of the system. The corresponding conclusions, however, may be biased due to limitations in the conceptual model. Specifically, the relative impact of fractures and the rock mass on bentonite hydration depends on the parameterization of the formation (see Section 4.4). A DFN that does not account for flow through the rock mass compensates for that fact by further increasing the transmissivity of the fracture network during the calibration process, thus giving rise to the notion that background rock flow is insignificant. Conversely, a model that overestimates background rock flow due to an artefact in the upscaling procedure may underestimate the importance of the fractures for bentonite wetting. See Section 4.9 for a related discussion.

- Model adjustments were made based on observed conditions and measured data from BRIE and WUT. As data generally became available before the modelling was performed, the modelling groups did not fully assess their model's ability to make reliable (blind) predictions in the absence of such detailed characterisation data. Considerably less information will be available when making siting decisions for deposition holes. Understanding the reliability of bentonite wetting predictions with limited characterisation data would have been valuable.
- To make discrete fracture network models better reproduce observed data, several adjustments of a different nature were made. These adjustments included a) conditioning the network to known fracture traces in deposition holes, b) calibrating fracture transmissivities and other properties, and c) picking the realisation that best matches observed inflow data. This flexibility in adjusting different DFN model components makes it relatively easy to match observed data. At the same time, it becomes difficult to avoid ambiguities and non-uniqueness that is inherent in an under-determined inverse problem. Furthermore, it is difficult to see which aspect of the fracture network (e.g. its geometry, or hydraulic properties, or spatial randomness) most critically affects bentonite hydration. Despite the stochastic framework adopted by DFN modellers, the uncertainty analysis lacks transparency. A detailed discussion of these fundamental issues would be most interesting.
- As BRIE testing and model development progressed in parallel, it would have been possible to assess the value of each additional data set assimilated in the model. Such an assessment (if done before data collection) could have been used to support or even optimise the design of BRIE. Even when done after data collection, the information could be used to guide the development of characterisation methods for deposition holes, which was one of the declared objectives of Task 8.
- The initial filling of the gap between the installed bentonite and the deposition hole wall, and an inadvertent flooding of the central tube led to a distinct transient signal in the observed relative humidities. Unfortunately, the modelling groups did not attempt to simulate the filling of the gap, despite it being a well-defined procedure with an accurately know amount of water being supplied. Moreover, the resulting transient response yielded a strong signal that likely contains valuable information about the bentonite's water absorption capacity without the uncertainty in the location and amount of water being supplied (as is the case for the natural inflow of water from the fractured rock). As a consequence of not simulating these events, the corresponding model results failed to reproduce the early-time data well, and there might have been a long-term effect because the simulated water balance did not include the additional water supplied to the system. When calibrating a model to measured data, it is essential to reproduce the test conditions with as high fidelity as possible to avoid a bias in the estimated parameters. In this particular case, not simulating the addition of water for gap filling is also a missed opportunity, as the perturbation generated valuable data that could have been used to constrain the model and estimate bentonite properties.

Calibrating a complex model using data of different type and quality is very time-consuming and challenging. While certain data may be well reproduced, others show either large or systematic residuals that are difficult to reconcile. Model calibration was not explicitly stated as a task, but data assimilation is implicitly encouraged as part of this exercise of developing a sequence of models that improve by the integration of field data that were collected with very similar overall objectives in mind.

The methods used to calibrate and condition a DFN (or hybrid models that are supported by a DFN) are interesting, as they address the difficult issue of concurrent parameter estimation and model structure identification. They also raise some fundamental questions about the appropriate level of model complexity, the relation between uncertainty and variability, and the relative importance of geometric and hydrogeologic properties.

None of the modelling groups employed a formal calibration method, where an objective function (within either a maximum likelihood or Bayesian framework) is minimized or mapped out using an appropriate minimization or sampling algorithm. The main disadvantage of not using a formal approach is not so much related to efficiency, but to the lack of an *a posteriori* error and uncertainty analysis that would provide considerable insights into the system behaviour and potential ill-posedness of the inverse problem. Nevertheless, some modelling groups commented on ambiguities, goodness-of-fit, the structure of the residuals, and their confidence in the estimates obtained by the calibration effort.

4.8 Comparison of performance measures

4.8.1 Background

One purpose of numerical simulations is to make quantitative predictions of a future system behaviour that cannot be readily inferred from historical data or from studying analogue systems. The numerical models developed as part of Task 8 were used to calculate a full set of independent and derived state variables at a large number of points in space and time. A small subset of these model outputs was identified as representing the system behaviour of interest, i.e. the quantities that most directly speak to the modelling objectives of understanding the exchange of water across the bentonite-rock interface and bentonite wetting, which may be related to criteria used for assessing the suitability of deposition holes. These outputs are termed "performance measures", and they naturally offer an opportunity to quantitatively compare the outcome of alternative conceptual and numerical models.

It is important to recognize that model predictions are inherently uncertain; this uncertainty should be accounted for when comparing simulation results.

The performance measures of interest are the inflows into probing and surrogate deposition holes as well as the time for hydrating the bentonite to a specific saturation level (typically 95 %). The following subsections summarize the values and (if reported) uncertainty ranges obtained by each of the modelling groups.

4.8.2 Inflow into open holes

Inflow into open boreholes was selected as a performance measure because it may be used as a screening criterion for the suitability of a deposition hole. Moreover, reproducing or predicting inflow may indicate whether a model reasonably represents flow processes in the fractured rock, with potential near-field modifications of properties. Estimating inflow is also essential as it determines water availability for bentonite hydration, and whether such wetting is controlled by the bedrock or by the bentonite water-uptake capability.

The modelling groups calculated inflow into open boreholes for a large variety of conditions, including inflow a) into large open tunnels, b) into small-diameter probing holes, c) into overcored surrogate deposition holes with enlarged diameters, d) with each hole opened individually, e) with all holes open simultaneously, f) with uncalibrated and g) calibrated models, h) with stochastically generated fractures intersecting the boreholes, i) with fracture networks conditioned to fracture traces observed in the boreholes, j) with increasing amounts of information available as the modelling work proceeded from Task 8C1 to 8D1 to 8F, and k) for variations in scenarios, cases, and parameters as part of the modelling group's chosen sensitivity analyses. Moreover, not all modelling groups reported inflows, or inflows are not reported in a complete or consistent manner. As a result, it is difficult to perform a formal, statistical analysis of the predicted inflows, or to find a common basis for comparing the results obtained by the individual modelling groups.

In general, most modelling groups adjusted their models to improve the fit to the measured inflows, including a) changing hydraulic properties of the fractures and rock mass, b) adding artificial features or zones around the boreholes, c) conditioning the fractures intersecting the borehole to measured data, d) screening DFN realizations for their ability to reproduce measured inflows, and e) changing other aspects of the model (e.g. boundary conditions, location and extent of large fracture zones, making assumptions about the fraction of water-conducting features or flow channelling within the fractures). Such adjustments are part of the model development process; they improve the understanding of the factors that affect inflow. The calibration or conditioning efforts undertaken as part of Task 8D1 considerably narrowed the spread of reported inflow predictions, both within and between modelling groups. For example, the groups reported mean or median inflows into Borehole 17 between 0.08 and 0.46 ml/min, with minimum to maximum inflows ranging from 0.0 to 30 ml/min. Notably, some of the modelling groups reported very narrow ranges, suggesting high confidence in their predictions, whereas others provided wide ranges. Again, it is difficult to compare these results; it is often unclear which uncertainties were examined to arrive at the reported ranges, or these ranges referred to analyses of different uncertain factors (e.g. the range arising by examining different realizations of the discrete fracture network, or by assuming lower and upper bounds on fracture transmissivity).

The following qualitative remarks are based on a consideration of the modelling groups' efforts to reproduce or predict inflows into open boreholes:

- It appears difficult to blindly predict inflows from a fractured rock into an open borehole.
- Models needed to be adjusted to reproduce measured inflows. These adjustments not only required static characterisation data (such as stochastic fracture properties or fracture traces used for deterministic conditioning of the fracture networks at each of the boreholes), but also dynamic data, such as pressures and – specifically – inflow data, i.e. exactly the type of data for which predictions are to be made.
- Prediction ranges were relatively large, even if the models were conditioned and calibrated. However, the prediction of inflow into an open borehole may not be as critical for the prediction of bentonite wetting, as long as the order of magnitude of the inflow correctly identifies the dominant regime (i.e. whether water supply from the fractured rock is below or exceeds the water-uptake capacity of the bentonite).
- Reported prediction uncertainties were difficult to interpret, mainly because the analyses used to obtain the ranges were done using constrained models, i.e. the ranges reflected only a subset of potentially influential, uncertain factors. Moreover, the basis for the reported ranges was not always clearly described.

4.8.3 Bentonite wetting times

Bentonite wetting time was selected as a performance measure because it is expected to be a key target prediction for numerical models that simulate the interaction between the natural and engineered barrier systems. The safety performance of the bentonite buffer partly depends on its swelling behaviour, which requires predicting the availability and uptake of sufficient formation water from the bedrock.

Most modelling groups predicted the saturation evolution in the bentonite. The importance of the location of fracture intersections (i.e. discrete inflow points) and the amount of water provided through the rock mass were universally recognized. The time until the entire bentonite buffer in a given borehole reaches a predefined average saturation was reported as the performance measure.

It proved difficult to compare the modelling group's prediction of bentonite wetting times and describe them using statistical tools, for reasons that are similar to those discussed in Section 4.8.2. Different measures were used (e.g. average saturation versus saturation at a specific depth), different saturation percentages were chosen as the threshold value to extract the wetting time, and different assumptions, features, and parameters were varied to examine the prediction range.

From the reported results, the following observations can be made:

- Bentonite wetting times were reported between less than one and more than 100 years.
- The range of wetting times reported by each modelling group is substantially narrower than the overall range obtained by combining the results from all modelling groups.
- All modelling groups reproduced the wetting time of the water-uptake test well. Predicting the idealized conditions of the WUT did not translate into similar wetting time predictions for the bentonite buffer in a larger deposition hole, which is highly determined by the location and geometry of discrete inflow points and water availability.
- The unique data set provided by the dismantling of BRIE significantly improved the fundamental understanding of the interface between the natural and engineered barrier systems. Nevertheless, quantitative predictions of the data collected at sensors placed within the bentonite proved challenging.

4.9 Comparison of main conclusions

4.9.1 Introduction

The main purpose of the Task 8 studies was to improve overall understanding of the water exchange between the natural and engineered barrier systems. Based on this improved understanding, secondary objectives can be achieved. In particular, characterisation methods are to be developed that help modellers improve their predictions of bentonite wetting times, which can then be used to establish deposition hole acceptance criteria. (Note that establishing the deposition hole criteria themselves was not part of the Task 8 scope.)

The following subsections summarise and compare some of the conclusions reached by the modelling groups regarding the main project objectives. As will be discussed, the modelling groups reached consensus on some aspects, and disagreed on others. It is not the purpose of this evaluation to arbitrate or make a determination about which conclusion is more viable. The purpose of this comparison is simply to present the range of alternative views and interpretations derived from a variety of conceptual and numerical models, which were developed based on a common set of data.

4.9.2 Dominant features

The system studied in Task 8 is complex. It consists of a geologic medium with fractures on multiple scales, from a) microcracks that may contribute to fluid flow through the rock mass, to b) small- and intermediate-sized fractures that can only be described statistically, to c) large deformation zones that need to be deterministically implemented in the numerical model. Embedded in this complex natural system are underground openings that range from boreholes to surrogate deposition holes to large tunnels. The presence of these engineered structures has changed both the properties of the geologic formation and the system state, specifically the pressure distribution and thus local and regional flow fields. Finally, the object of interest is a deposition hole filled with an initially desaturated clay material. Installation of bentonite in a borehole excavated in a fractured rock leads to interactions between the engineered and natural barrier systems. The topic of Task 8 is to study this interaction.

Both the natural and engineered systems have to be abstracted to reduce their complexity and to make them tractable for scientific analysis and numerical modelling. This abstraction process deals with the question of which features, events, and processes (FEPs) have a potential impact on the system behaviour and thus need to be accounted for in the numerical model. Identifying the key elements is part of model development itself and is thus an iterative process.

Task 8 was designed such that iterative model updating is an integral part of the exercise. Specifically, the amount of data from BRIE increased during the course of the project, allowing the modelling groups to test their hypotheses and revise their models. Mismatches between numerical predictions and observations may point towards aspects of the model that need to be refined. Conversely, sensitivity analyses may suggest that certain features can be omitted or simplified without loss of the model's ability to make reliable predictions.

The relative importance of each feature defines the level of accuracy with which their characteristics need to be determined and the effort spent on faithfully representing them in the model. System understanding is essentially a description of those features and processes that are believed to be critical for making inferences about the observed or future system behaviour.

The following is an (incomplete) list of features that were discussed as being potentially significant for predicting bentonite hydration:

- Far-field boundary conditions.
- Initial conditions, specifically in bentonite.
- Large discrete geologic structures and deformation zones.
- Stochastic fracture network.
- Fractures intersecting boreholes and tunnels.
- Rock mass between fractures (including unmapped microfractures).
- Underground openings.
- Skin zones around underground openings.
- Interface between fractured rock and bentonite.
- Bentonite properties, specifically water absorption capacity and related swelling behaviour.

Within each of these categories, questions may be asked regarding the relative importance of the feature's various properties. For example, there is general agreement that fractures play a key role in determining water availability for saturating the bentonite as well as the flow pattern at the bentonite-rock interface, which critically affects wetting time. However, it is less obvious which of the large number of properties characterising fractures and fracture networks are most influential. Some of the subcategories and properties to be considered include:

- Large deterministic geologic structures control large-scale flow and pressure fields and water availability near deposition holes.
- Intermediate-scale fractures provide connectivity from boundaries and large features to the deposition holes.
- Small- and intermediate-scale fractures intersecting the deposition hole determine water inflow rate and wetting pattern, which influences bentonite wetting times.
- Microfractures contribute to rock-mass permeability and promote a spatially more distributed wetting of the bentonite a lower rates, as opposed to localized inflow from larger fractures at higher rates.
- Transmissivity and heterogeneity of individual fractures determine hydraulic activity and flow channelling and thus probability, geometry, and amount of water supplied to a deposition hole.
- The structure of the stochastic fracture network (i.e. number, density, shape and stochastic distributions of location, orientation, and fracture size) determines connectivity and effective properties of the fracture network.
- Hydraulic behaviour across fracture-matrix contact areas and along fracture intersections affect flow patterns in the bedrock and at the bentonite-rock interface.
- Two-phase properties of fractures and the rock mass determine effective permeabilities, desaturation behaviour and gas trapping near the bentonite-rock interface.
- Stress redistribution near underground openings and related deformations determine near-field flow patterns and hydraulic properties of the key fractures intersecting the deposition hole.

Sections 4.3 to 4.6 describe the different conceptual models that were developed by the modelling groups based on their respective understanding and different prioritisations of key features. Key features were selected based on experience and prior knowledge of similar systems (at the Äspö Hard Rock Laboratory and elsewhere), but also because of the capabilities of the available simulation software. Most modelling groups then conducted sensitivity analyses to determine which of the features and/or a feature's properties most significantly influence inflow into deposition holes and bentonite wetting. As mentioned before, these sensitivity analyses were confined to each group's chosen modelling framework; the conclusions reached by the modelling groups often reflect these constraints imposed by the modelling framework.

There was general consensus about the importance of the following features:

- Number, location, orientation, and properties of the discrete, water-conducting fractures that intersect the deposition holes have a high impact on wetting patterns and bentonite hydration times. Mapping these fractures and deterministically implementing them correctly into the model is essential for reliably predicting bentonite wetting.
- The bentonite properties, specifically sorptivity (permeability and water retention curve) are key parameters. It seems to be possible to characterise or infer these properties with sufficient accuracy in the laboratory (e.g. through a water-uptake test).

The second group of factors is related to the means by which water is carried to the deposition hole. The modelling groups' opinion on the relative importance of the fracture network versus that of the rock mass reflects the chosen conceptual model:

- The modelling groups that developed a DFN considered the structure of the fracture network to be an essential component of the system that needs to be well understood to properly capture connectivity and water availability. These features are described using stochastic concepts; they thus have a random component that reflects spatial variability. It is noteworthy that this randomness is removed (even though the statistical metrics are preserved) at the interface itself, where mapped fractures are inserted deterministically to condition the DFN.

- The modelling groups that developed a (homogeneous or heterogeneous) effective continuum model or a hybrid model (with discrete fractures intersecting the deposition holes) concluded that the details of the far-field fracture network structure is of limited relevance and can thus be subsumed into a simplified continuum representation. Characterisation of the far field thus can be limited to a few effective properties that capture the formations ability to provide water to the region immediately surrounding the deposition holes. The hybrid approach also allowed the modellers to include the effects of unmapped (small) fractures.
- For dry sections of deposition holes that are not intersected by water-conducting features, the permeability of the rock mass (which may include microfractures) was considered important. Modelling groups that used a classical DFN implicitly screened out the rock mass as an influential feature. Note that while the influence of small fractures was acknowledged, the length scale below which fractures (and the matrix) were neglected was determined by the threshold value used during fracture-trace mapping. Practical limitations determine this threshold value rather than a consideration of the impact of small fractures on bentonite wetting.

The third group of factors includes features that most modelling groups considered of limited importance. Most groups reached this conclusion after performing sensitivity analyses, or they excluded the feature in an initial screening step:

- The large discrete geologic structures (deformation zones) were generally considered of limited influence as long as they do not directly intersect a deposition hole or tunnel.
- Skin zones around underground openings were considered proxies for changed fracture and background rock properties (see discussion above).
- The interface between the bentonite and the fractured rock was not explicitly considered in the modelling. It can be assumed that its effect on the exchange of water from the natural to the engineered barrier system was considered irrelevant. Implicit assumptions about the interface were made, but these assumptions were neither described nor tested.
- The details of the far-field boundary conditions were considered insignificant as long as they provided water and pressure support to the fractures carrying water to the deposition holes.

Finally, some of the modelling groups focused their studies on specific aspects or properties. For example:

- Gas trapping in the bentonite, if included in the model, was considered important for determining the time until the bentonite reaches full saturation.
- Bentonite wetting was critically determined by a simple classification, which is the ratio between water supply from the rock and water demand by the bentonite.

As shown in this subsection, the modelling groups reached some consensus regarding the fact that bentonite wetting is foremost determined by a) the bentonite properties, and b) the local properties of the fractures in the immediate vicinity of the deposition holes. On the other hand, there are different prioritisations of features or contradicting conclusions regarding the relative importance of the fracture network structure and rock mass.

Both the agreements and discrepancies have to be considered when deciding what characterisation data are to be collected to improve the reliability of model predictions of bentonite wetting and ultimately deposition hole siting.

4.9.3 Reliability of model predictions

The modelling groups' confidence in their predictions of bentonite wetting rests to a large degree on the favourable reproduction of data from the water-uptake test and from the results of Task 8F, which showed that relative humidity data measured in the bentonite after BRIE dismantling can be reasonable well matched. It should be noted, however, that matching these data required detailed information (and sometimes corrections) of fracture and sensor locations, and that the comparisons were sometimes limited to certain areas in the bentonite (e.g. only close to fracture intersections, or only to dry or wet segments, or only close to the rock-bentonite interface). Blind predictions or calculations based on fewer characterisation data may thus be less reliable.

Non-uniqueness in the parameter values or scenarios was recognized by some of the modelling groups, specifically when applied to the prediction of inflow into open boreholes. The question arises whether such ambiguities in the representation of the natural system are essential and prevents the reliable prediction of bentonite wetting times. This issue will be discussed in the following subsection.

4.9.4 Bentonite wetting controlled by natural or engineered barrier system

The complexity, multi-scale heterogeneity, and inaccessibility of a natural underground system lead to considerable uncertainties in its characterisation and the subsequent model predictions. As amply demonstrated in Task 8, the apparently simple calculation of inflow into an open borehole faces considerable challenges and results in a very wide range of predicted rates despite detailed data from fracture mapping, hydraulic testing, and monitoring. Assessing and documenting input, estimation, and prediction uncertainties is essential. An uncertainty analysis is the first step in assessing the reliability of model predictions and the conclusions drawn from such simulations. Note that while prediction uncertainty may be high, this does not necessarily indicate that the host rock of a real repository is not effective as a natural barrier.

The engineered barrier system is generally easier to characterise and to predict, mainly because a) it is a system designed by humans, b) its components can be fabricated according to specifications, and c) it can be tested in the laboratory or in specially design field experiments (such as BRIE). While in itself highly complex, bentonite is used as a material in engineered barrier systems of a nuclear waste repository partly because of its self-healing and homogenisation properties, which are expected to reduce the variability and uncertainty imposed by the natural system.

Both the natural and engineered systems have overlapping and complementary barrier functions (most of these functions were not the subject of this project). Nevertheless, Task 8 investigated the interaction between the two barrier systems, specifically whether the water supplied from the fractured rock sufficiently saturates and swells the bentonite so that it can assume its barrier function. A key finding of the modelling studies was that the bentonite-wetting pattern is highly heterogeneous as a result of the discreteness of inflow from the fractured rock. Swelling is thus non-uniform, and the homogenisation function of the bentonite may – at least at early times – not be fully realised.

Some modelling groups interpreted this finding as a strong need for an accurate characterisation of the fractured rock, as it dominates the inflow pattern. The following statement concisely summarizes this view:

"*The modelling shows that the stochastic fracture network has a large impact on the wetting process.*"

The scale on which fracture characterisation data are needed, and whether these fractures must be included deterministically or stochastically, or whether they can be represented by effective rock-mass properties, are questions that are only partially answered.

Other modelling groups concluded that bentonite hydration is predominantly controlled by the (well-known) bentonite properties, and that the characteristics of the natural system are secondary as long as the fractures intersecting the deposition holes are properly mapped and deterministically incorporated into the model. The conclusion that the natural system is of secondary importance is significant: it allows investigators to focus their characterisation efforts on a few key properties rather than having to embark on an extensive mapping and testing campaign to reduce all uncertainties inherent in a natural system. The following two statements concisely summarize this view:

"*Large-scale, complex models of the natural system have low predictive significance for bentonite wetting.*"

"*The modelling shows that we are able to reproduce the wetting rather well despite a rather coarse treatment of the surrounding rock.*"

As indicated above, not all modelling groups share this view. It is therefore essential to further examine this issue and assess under which conditions either of the two views voiced in Task 8 may be valid. Another view may be formulated, stating that bentonite wetting is being driven by a) the bentonite properties, and b) by *local* properties of the fractured rock.

It is important to note that siting criteria for deposition holes are concerned with many aspects other than bentonite hydration. For some of these additional considerations, the properties of the bedrock are unquestionably significant, i.e. an accurate characterization of the natural barrier system is certainly needed in support of deposition hole siting decisions. This broader context of deposition hole siting must be considered when interpreting the statements and conclusions made in this report.

4.9.5 Characterisation needs

Characterisation needs are determined by:

- The overall objectives of a project (e.g. improve the reliability of deposition-hole siting decisions; note that the overall objectives also determine the scale and relevant processes).
- The understanding about which features or properties have the largest influence on the key model predictions that are made to support the ultimate project goal.
- The accuracy with which these predictions need to be made.
- The current uncertainty of the key feature's properties.
- The model structure (characterisation data are used to determine parameters that are always related to the given model structure).

This list clearly indicates that the prioritisation of characterisation needs is driven by a) the overall understanding of how the natural and engineered barrier systems interact with each other, and b) by the ranking of (uncertain) features that control bentonite wetting. As discussed in the previous sub-sections, no unanimous conclusion regarding the key factors affecting bentonite wetting was reached. While the importance of fractures was recognized, it remains unclear which fracture characteristics need to be determined with high accuracy, and how they may be best included in a numerical model. Practical limitations (e.g. feasibility of detailed mappings of inflows or fractures intersecting probing holes) also need to be considered.

Despite some differences in the modelling groups' detailed views, it appears necessary to have sufficient characterisation data of a) the bentonite's water-uptake properties (essentially permeability and capillary strength), and b) geometric and hydraulic properties of the local fractures intersecting the deposition hole. At the Äspö Hard Rock Laboratory, the network of intermediate-scale fractures seems sufficiently connected to provide water to the deposition holes in amounts exceeding the demand of the bentonite; consequently, a simplified representation of the far field appears justified at this specific site.

5 Concluding remarks

5.1 Summary

This evaluation report first described the original intent and structure of Task 8 (Section 1), which is followed by a summary of the work done by the 11 modelling groups (Section 2). Section 3 then provided a short evaluation of each modelling group's results with respect to each subtask's objectives. In Section 4, some key aspects of the Task 8 scope were examined in a preliminary comparative analysis, which discussed similarities and differences between the pool of alternative conceptual models provided by the modelling groups rather than looking at results within each group's framework. This perspective may lead to additional insights, as discussed in Finsterle et al. (2018).

Task 8 is conceived primarily as a modelling exercise. The following subsections contain some final thoughts on model-related issues.

5.2 Conceptual models

One of the most beneficial outcomes of Task 8 is the large number of alternative conceptual models that were developed to address a common issue based on a common set of characterisation data and background information. The variety of approaches taken to assess the interaction between the fractured rock and the bentonite buffer in a deposition hole led to insights and conclusions that a) can be considered robust in cases where different groups converged on a consistent understanding, and b) highlight fundamental uncertainties, ambiguities, or lack of defensible understanding in cases where opposing views were held despite the common information available to and shared among the modelling groups. Both of these insights are considered equally valuable.

The modelling groups documented their respective conceptual models with different levels of detail and scientific rigor. Therefore, the following critical assessment of the conceptual models developed as part of Task 8 does not refer to the work of a specific modelling group, but summarizes some general observations.

- Conceptual models were generally developed within the framework and constraints of the available simulation tools rather than based on a critical assessment of key features, events, and processes that potentially affect groundwater flow through the fractured rock, across the rock-deposition hole interface, and into the bentonite.
- Most modelling groups focused on a single conceptual model; consequently, no formal evaluation of conceptual modelling errors could be made.
- Many modelling groups strictly adhered to the information provided in the task description. A critical assessment of this information prior to its implementation in the model is recommended.
- The modelling reports did not contain a detailed description of the rock-bentonite interface, the features of this interface, the relevant processes occurring within this interface (see Section 4.6 for a partial list), and the feedback mechanisms between the natural and engineered systems. This omission is unfortunate given that the topic of Task 8 was the interaction between the natural and engineered barrier system across that interface.
- Abstraction steps were not always justified in a transparent manner, including those regarding the fundamental representation of the fractured rock as well as the coupling between the natural and engineered subsystems. Abstraction steps were well documented by modelling groups that employed a hybrid approach.
- Newly available data from BRIE and related property adjustments did not trigger fundamental changes of the initially defined conceptual models.
- Different aspects of a given model were represented with different levels of detail and complexity. The chosen level of complexity is not clearly linked to the relevance of that aspect.
- Conceptual models were not clearly linked to hypotheses to be tested.

As stated above, multiple alternative conceptual models were developed as part of Task 8, which provided a unique opportunity to examine conceptual model uncertainty. Such a comparative analysis, however, requires each group to take a step back and look at the combined work of all modelling groups. While such a perspective was assumed by many of the participants during the Task Force meetings, it did not result in corresponding discussions in the modelling reports, which focused on the specific model developed by each group.

Assessing the conceptual model and testing hypotheses can be viewed as improving system understanding, which is a declared goal of Task 8. Considerable steps towards that goal have been made as part of Task 8, specifically in the final Subtask 8F.

5.3 Role, characterization, and representation of fractures

The importance of fractures for understanding and predicting fluid flow and bentonite hydration is universally recognized. Nevertheless, there remain considerable differences in the assessment of which properties of fractures and fracture networks are most essential, how to best characterize them, and how to properly include them in a representative and efficient manner in a numerical model. The differences in the modelling groups' view are essential, as they determine the choice of (potentially costly) characterization methods and modelling approaches.

Many of these issues have been discussed throughout this report; they are not repeated here, with the exception of the question about the representativeness of fracture trace maps. The roles of fractures smaller than the mapping threshold length as well as microfractures are recognized, with different approaches used to represent them in the numerical model (see discussion in Section 4.4).

A second issue of importance is the ratio of fractures that are expected to contribute to fluid flow. Some modelling groups saw the need to (considerably) reduce the number of fractures to account for hydraulically inactive fractures. Without such an adjustments, inflows into open holes are significantly overestimated. Others referred to the observation that fracture locations and orientations seen in the bentographs are generally consistent with the fracture statistics used to generate the DFN. They then concluded that most of the geologically mapped fractures have the potential to provide groundwater to the bentonite even if their permeability is lower than the detection limit of the hydraulic investigation.

5.4 Interaction with BRIE

Task 8 was predominantly devised as a numerical modelling exercise. However, it also offered the great opportunity a) to support the design of BRIE by optimising the experimental layout and monitoring system by predicting the expected system response, b) to analyse the measured data to improve system understanding, c) to calibrate the models and test hypotheses, and d) to assess the reliability of the model predictions.

The active participation of the BRIE experimentalists in Task 8 is considered highly valuable. Data from the water-uptake test provided confidence in the model representation of bentonite, and data from the dismantling of BRIE provided direct evidence of flow patterns across the rock-bentonite interface as well as quantitative measures of bentonite wetting.

Nevertheless, the benefits from close collaboration and exchange of information obtained from field activities and related modelling studies could have been higher. It would have required good coordination between the two activities and a clear formulation of hypotheses and goals of mutual interest that can be addressed by collecting specific data that are predicted and analysed by numerical modelling.

Suggesting a more comprehensive analysis framework with a clear request to continually assess uncertainties would have helped streamline the modelling work so it could have evaluated the usefulness both existing data as well as potential data that could be collected as part of BRIE to improve system understanding or help determine values and statistics of parameters that most influence the model predictions of interest. Finally, it would have focused the modelling more on hypotheses testing and thus improved system understanding.

5.5 Model calibration

The process of conditioning and calibrating a model links it to site-specific conditions as represented by observations of the system behaviour at discrete points in space and time. A systematic misfit between model and data may point towards aspects of the model that may need to be refined. These may be specific features or parameters, but also include conceptual aspects or hypotheses. To make model testing more stringent, it would be desirable to discuss or even quantify modelling and data errors, so that an objective calibration target can be defined. This assessment of the expected residuals has to be done prior to model calibration to serve its purpose. It would also require that input uncertainties be quantified and propagated through the model, so that the uncertainty in the predictions can be compared to the acceptable uncertainties as demanded by the study objectives. Such a comprehensive framework was not envisioned at the beginning of the Task 8, and was thus not formalized. An attempt was made towards the end of the project, when modelling groups responded to the uncertainty questionnaire (see Section 1.7 and Appendix A), documenting their conceptual thinking.

5.6 Modelling in support of application-driven system understanding

As discussed in Section 5.4, including field experimentation into a combined EBS and GWFTS SKB Task Force exercise provided a unique opportunity to improve application-driven system understanding, because the studies were linked to the specific configurations, conditions and realities of the bentonite-rock system of interest.

5.7 Decision making based on models and data

The work performed as part of Task 8 may inform criteria to be used in deposition hole siting decisions related to bentonite buffer performance. While no such criteria were formulated as part of Task 8, it became evident that siting decisions will need to be based on both local characterisation data and some (potentially simplified) predictive modelling. The degree to which siting decisions rely more on measured data or model predictions may change with scale. Ultimately, the importance of being able to develop robust criteria depends on the impact that bentonite wetting patterns and time has on overall system performance.

5.8 Natural system – engineered system

Task 8 was concerned with the interaction between the natural and engineered barrier systems. Some of the analyses suggested that bentonite wetting is controlled by only one of the two considered subsystems: Bentonite wetting may be limited by the amount of water supplied by the fractured rock, or by the water-uptake capacity of the bentonite. The properties of each subsystem in relation to those of the other determine whether a controlling factor can be uniquely assigned to one of the two subsystems. If so, characterisation efforts could be focused. However, it should be recognized that discrete inflow patterns (which are controlled by the fracture network) strongly influence bentonite wetting even if the water-uptake capacity of the bentonite is the hydraulically controlling factor. A good understanding of the natural system, its variability and uncertainty remains essential. It is also recognized that each of the two subsystems considered in Task 8 has multiple barrier functions; saturating the bentonite around the waste packages is one, albeit important, prerequisite for some of the buffer's barrier functions.

5.9 Overall evaluation

As stated in the task description (Vidstrand et al. 2017), the "objective of the task and the joint field experiment BRIE (Bentonite Rock Interaction Experiment) was that these would lead to: i) a scientific understanding of the exchange of water across the bentonite-rock interface; ii) better predictions of the wetting of the bentonite buffer; and iii) better characterization methods of the canister boreholes".

The benefits of Task 8 may be evaluated differently by the participating individuals, modelling groups, supporting organisations, sponsors, nuclear waste agencies, the scientific community, or the concerned public. From the perspective of the appointed reviewer, the following overall evaluation comments are based on the specific evaluations summarized in Sections 3 and 5.2 through 5.8:

- *The work of the Task 8 modelling groups contributed to an improved understanding of the factors that affect the wetting of the bentonite buffer in deposition holes emplaced in fractured granitic rock. These insights were gained with support from data collected during BRIE and the related water-uptake tests. While the modelling groups arrived at different views about some aspects of the system, both their agreements and differences led to an improved overall understanding.*
- *The value of the modelling work could be further increased by examining the numerical results with focus on specific hypotheses that were (or need to be) formulated to better understand bentonite-rock interactions.*
- *The Task 8 work developed conceptual models, simulation tools, approaches and workflows that can be used to effectively target scientific questions of practical relevance for nuclear waste disposal in buffered deposition holes. Now that the tools are available, future studies may focus more on the interpretation of the modelling results.*
- *The exchange of information and discussions during the Task Force meetings and workshops were dynamic, friendly, and professional, providing a solid basis for the overall success of Task 8.*

5.10 Recommendations

The following recommendations are made:

- A conscious decision is to be made about how prescriptive a task description should be. This decision should be based on the technical objectives, but also accounting for the concept and goals of the Task Force as a whole.
- In the Task Force, multiple modelling groups address the same issues related to the interaction between the natural and engineered barrier systems. However, these issues were examined based on the group's specific areas of expertise and using different conceptual models, methods, tools, and interpretations. Moreover, the modelling groups (with one exception) provided results for only a subset of the tasks, which further reduced the overlap among the individual studies. For the Task Force to become more than a collection of individual modelling studies, it would be very valuable to encourage the groups to participate in a comparative analysis that provides a new perspective on broader lessons learned, unresolved issues, and conceptual uncertainties. It is recommended to make this comparative analysis an integral part of the Task Force by explicitly including it in the task description. For example, each group would dedicate a member to collaborate with the other modelling groups on the comparative analysis from the beginning of the project. The responsibilities of this member would be to interact with his/her counterparts from the other modelling groups during the year, informing the rest of his/her team about progress and decisions, and coordinating the team's efforts to provide the information needed for the comparative analysis. A special session could be organized during TF meetings (e.g. parallel to the executive session) to discuss integration issues. Making a comparative analysis an integral part of the Task Force would have the following advantages:
  - Project objectives would be clearly articulated, and a list of testable hypotheses would be formulated.
  - The conceptual model and associated modelling assumptions would be clearly documented and communicated to the other modelling groups.
  - The risk that working towards a comparative analysis would lead to a more uniform set of alternative conceptual models could be mitigated by requiring that models deviate from each other by at least one key conceptual assumption. These differences could then be examined and used to discriminate among competing hypotheses, to the benefit of all modelling groups.
  - Modelling groups may also be encouraged to jointly examine a particular issue where concepts and modelling capabilities complement each other.

- The need for informative and robust performance measures would be apparent, and modelling results would be documented in a concise and complete manner.
- The basis for a broader sensitivity analysis could be created.
- Insights into the relative importance of data, parametric, and conceptual model uncertainties would be gained.
- Modelling results would be interpreted and conclusions would be drawn with a more focused view on the common, overall objectives.
- Participation in an overarching comparative study would encourage collaboration and information exchange among the modelling groups. It may also motivate timely reporting of modelling results.
- Comparative analyses may lead to well-cited publications in the scientific literature.

• The Task Force projects are placed within the context of nuclear waste disposal. Uncertainty is an inherent aspect of this area of science and technology, regardless whether a specific Task Force project is concerned with research of fundamental processes, site characterisation, or performance assessment. Uncertainty (its description, quantification, and propagation) should thus be an integral part of the project from its beginning, with related guiding questions explicitly included in the task description. An example of such guiding questions can be found in Appendix A.

• A strong link between numerical modelling and laboratory or field experimentation is of great value. Both activities benefit from each other if one part of the modelling is dedicated to supporting experimental design, and if testing and monitoring generate data that help a) calibrate the models, b) discriminate among alternative conceptualisations, and c) test hypotheses. A successful interaction between numerical modelling and physical experimentation requires considerable planning and coordination, and the willingness to adjust one's work scope to support the other group. Such cooperation may be facilitated by the Task Force Secretariat and outlined in the task description.

• If considered helpful and with the consent of the modelling groups, an annotated outline of the final modelling report could be provided early on. One might consider making this outline follow the general structure of a research paper (rather than that of a project report) to facilitate and encourage publication of the Task Force work in the scientific literature.

• A lecture or seminar by an outside expert on a topic of relevance to the Task Force work could be useful and stimulating. This expert may also be willing to participate in parts of a Task Force meeting and provide feedback.

This report has been reviewed by the modelling groups and the SKB Task Force management. However, the opinions and specifically the evaluation comments are those of the author.

6 Acknowledgement

I first want to thank Gunnar Gustafson, who gave me the opportunity to participate in the Task Force as the evaluator; I miss Gunnar as the leader of the Task Force, colleague, and friend. From the very beginning, Bill Lanyon guided me through the Task Force evaluation process; his thoughtful advice on all technical and administrative aspects was invaluable and is greatly appreciated. I want to thank SKB for hosting the Task Force, and for its financial and logistical support over many years; I very much enjoyed working with Björn Gylling of the Task Force Secretariat. Finally, it was a great pleasure to get to know the colleagues participating in Task 8; I thank the members of the modelling groups for sharing their work and insights, and for making my job as the evaluator interesting, challenging, and rewarding.

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Appendix A

A framework for comparative analyses and conceptual uncertainty evaluation

SKB Task Forces on
Modelling of Groundwater Flow and Transport of Solutes and Engineered Barrier Systems

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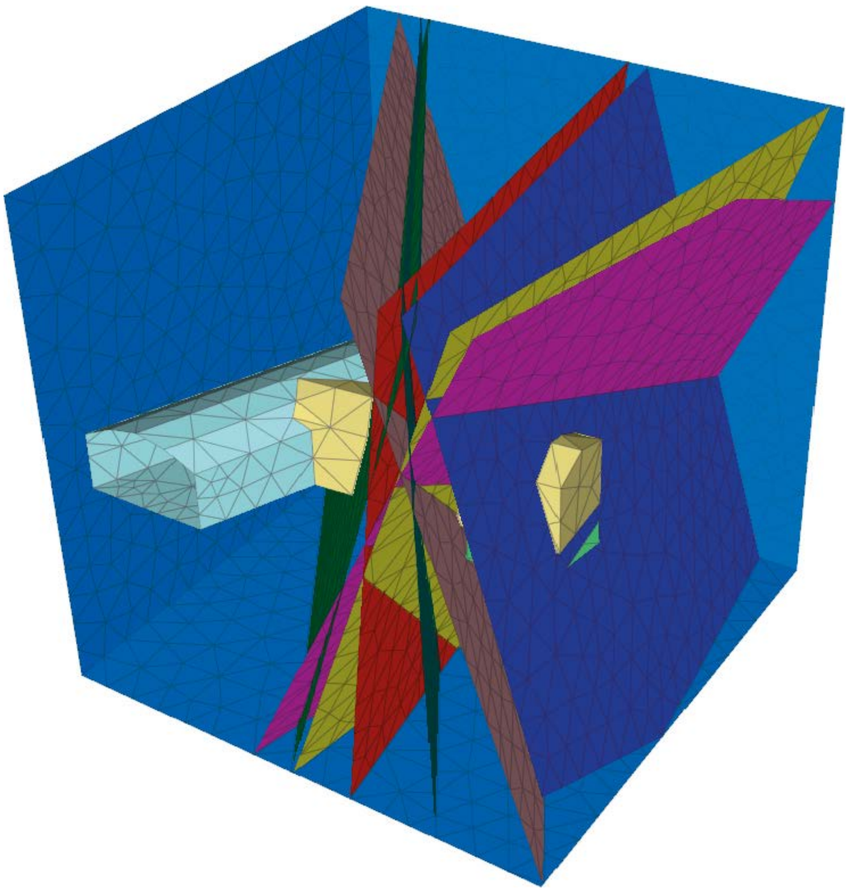

Keywords: Äspö Hard Rock Laboratory, SKB Task Force, conceptual model, numerical analysis, uncertainty analysis

This report concerns a study, which was conducted for SKB. The conclusions and viewpoints presented in the report are those of the authors and do not necessarily coincide with those of the client.

A1 Introduction

A1.1 Background

The SKB Modelling Task Force is a forum for the international organizations supporting the Äspö Hard Rock Laboratory to interact in the area of conceptual and numerical modelling of groundwater flow and solute transport in fractured rock as well as of engineered barrier systems.

Task 8 is a joint effort of the SKB Task Force on Modelling Groundwater Flow and Transport of Solutes (GWFTS) and that on Engineered Barrier Systems (EBS). The overall objective of the task is to obtain a better understanding (through modelling and analyses) of the hydraulic interaction between the near-field bedrock and backfill materials in the repository, specifically the bentonite buffer in a deposition hole.

A1.2 Status and opportunity

Each of the modelling groups participating in Task 8 developed a conceptual and related numerical model of the system, whose general outline was defined in the task description (Vidstrand et al. 2017). While each group essentially focused on a single conceptual model, the project as a whole produced results that are based on a suite of alternative conceptual models. Initial evaluation of the project reports indicates that

1. the choice of the conceptual model seems partly driven by the capabilities of the simulator available for the analysis, rather than an evaluation of potentially influential features, events, and processes;
2. the majority of the simplifications and assumptions that underlie the chosen conceptual model are presumed valid rather than formally tested;
3. sensitivity analyses conducted by the individual modelling groups are limited to the confines of the chosen conceptual model and its parameterization;
4. uncertainty analyses conducted by the individual modelling groups mostly examined the impact of parametric uncertainties; conceptual uncertainties were not evaluated, and
5. conclusions reached by the individual modelling groups are naturally related to the features of the conceptual model.

Points 2–5 are general limitations of any analysis that is based on a single conceptual model. Nevertheless, documenting the decisions made during conceptual model development and associated uncertainties are essential when trying to gain improved system understanding, which is the overall objective of Task 8. The fact that multiple models of the same repository subsystem are available provides a unique opportunity to examine conceptual model uncertainty.

A1.3 Objective

The objective of this document is to propose a process that enables a comparative analysis of modelling results and evaluation of conceptual model uncertainty. This proposal has to account for and is limited by the specific circumstances of this SKB Task Force project, including its status, currently available or expected information, and time constraints.

A1.4 Short literature review

The (often dominant) impact of the conceptual model on simulation results is widely acknowledged (the examples described by Bredehoeft (2003) are illustrative). As a consequence, various methods have been proposed to:

1. gain confidence in the appropriateness of the chosen conceptual model;
2. rank the performance of alternative conceptual models;
3. identify plausible models or select the most appropriate model;
4. average multiple models to obtain consensus predictions;
5. quantify the sensitivity of model outputs to changes in the conceptual model;
6. quantify uncertainty in predictions as a result of conceptual model uncertainty, and
7. guide future data collection and modelling activities.

Papers published in the scientific literature range from philosophical discussions (e.g. Pappenberger and Beven 2006) to qualitative descriptions (e.g. Marivoet et al. 1997), empirical studies (e.g. Bredehoeft 2005), and to quantitative theories (e.g. Neuman 2003). In hydrogeology, most of the literature related to conceptual uncertainty revolves around the generalized likelihood uncertainty estimation (GLUE) method (Beven and Binley 1992), Bayesian model averaging (Draper 1995), the use of model selection criteria (Ye et al. 2008), and combinations thereof (Rojas et al. 2010, Ye et al. 2010, Singh et al. 2010). A few papers describe conceptual model comparison studies for specific application areas, including nuclear waste isolation (Baca and Seth 1996, Marivoet et al. 1997, Rutqvist et al. 2009, Hudson et al. 2009, Reeves et al. 2010, Li et al. 2011). Many more studies focus on benchmarking and code comparisons (e.g. Oldenburg et al. 2003, Pruess et al. 2004, MDH 2005, Steefel et al. 2015); they often do not fully include uncertainties caused by the process of developing a conceptual model from available information. Conceptual model uncertainty has been discussed as part of international code and model comparison projects, such as INTRAVAL, INTRACOIN, HYDROCOIN, PSACOIN, DECOVALEX, CO2BENCH, SSBENCH.

Without going into the details of the proposed approaches, the following observations can be made:

1. Identification of the true (or even most likely) conceptual model is considered impossible (Oreskes et al. 1994).
2. Multiple (if not many) conceptual models need to be developed (or conceptual aspects of a model need to be parameterized) for a suitable analysis.
3. Measured data are often required to calibrate the model or to evaluate its performance (Pappenberger et al. 2015).
4. Estimates of prior model probabilities and input parameter uncertainties as well as their impact on predictions are often required as part of a formal conceptual model uncertainty analysis.
5. A suitable likelihood measure needs to be defined and evaluated for each alternative conceptual model.
6. Most approaches involve computationally expensive Monte Carlo sampling methods (Rojas et al. 2010).
7. Model performance is most often evaluated in the calibration rather than prediction space (Poeter and Anderson 2005).
8. Correlations among alternative conceptual models are seldom accounted for (a notable exception is Sain and Furrer 2010). As model-to-model correlations are likely very strong, this may discard the use of simple methods such as bootstrapping.

Many of the requirements stated in these observations make it difficult to formally evaluate conceptual model uncertainties without a careful design at the beginning of such an analysis so a retrospective application is not without problems. However, the Task 8 modelling has been conducted in tandem with the BRIE field experiment, and data from the laboratory water-uptake test are also available. Moreover, in addition to the general goal of improving system understanding, Task 8 defines some specific prediction targets which can be used as performance measures for the purpose of an uncertainty analysis (although that was not the original intention). The use of specific target predictions is also a means to limit the scope of the uncertainty analysis, which otherwise extends to include the challenging issue of using models calibrated against short-time experimental data for use in assessments for long-term repository performance.

A2 Proposed approach

A2.1 General idea

Task 8 provided a rather wide range of models, which we may consult in forming views on the repository system behaviour. These models have different levels of accuracy as well as overlapping (but not identical) input spaces, which arise from sharing the task description and some common aspects of the underlying conceptual understanding. Synthesizing the results of these alternative conceptual models requires some evaluation of the prediction uncertainty that includes conceptual, parametric, and numerical errors and their correlations.

Such a formal evaluation, however, is beyond the scope of what can be accomplished within this project. Instead, we propose to discuss conceptual model uncertainty in a qualitative rather than quantitative manner. Nevertheless, the discussion is intended to be as specific as possible in that it focuses on the repository subsystem at hand, the hydrogeological features of that subsystem, the numerical models that were developed as part of Task 8, and the target predictions these models were asked to deliver.

To guide such a discussion, we propose to collect specific information from each of the modelling groups as the basis for a comparative analysis. Most of the requested information consists of a concise and complete documentation of each modelling group's system understanding, the features implemented in their models, the explicit and implied assumptions made during model development, and the modelling group's assessment of the validity and uncertainty of these assumptions. In addition, results from the sensitivity analyses conducted by most modelling groups and more general valuations of the quality of model predictions should be summarized. These descriptions may be supplemented with results from numerical simulations or estimated measures of prediction uncertainty.

(It should be noted that it is essential to define the intended use of a model before identifying the key target predictions and evaluating the model's performance. Specifically in models used to assess the long-term safety of a nuclear waste repository, prediction models are often extrapolated far beyond the conditions, processes, spatial and (specifically) temporal scales of the models used for calibration or comparison with experimental or monitoring data. While addressing this issue and the question of how the performance of a model can be evaluated as it supports the ultimate goal of nuclear waste isolation, we focus here – as described above – on the limited modelling goals as outlined in the task description.)

The following subsections further describe the approach and provide a list of information considered essential for an evaluation of conceptual model uncertainty. This list is eventually presented in the form of questions or an annotated outline, which the modelling groups may consider as a template for their reporting.

A2.2 True system, reified model, and actual model

It is understood that conceptual model errors are an inherent part of numerical modelling, as building a model involves an abstraction process during which certain aspects of the real system are simplified. To become more aware of this abstraction process and, furthermore, to highlight the further simplifications made when implementing the conceptual model into a numerical model, we propose to make use of the concept of a "reified model" (Goldstein and Rougier 2009). A reified model is simply the "best conceivable model" a user would develop without being constrained by computational limitations (such as CPU time and memory). Defining such a hypothetical model allows one to separate potential errors made during the abstraction step and those made during the implementation step. Note that the difference between the true system and the reified model reflects our incomplete knowledge of the system behaviour, whereas the difference between the reified model and the actual computer model used for an analysis reflects modelling deficiencies (including effects from data uncertainties). The first discrepancy is fundamentally not knowable, even though measured data may give us a (also erroneous) glimpse of what the true system behaviour might be. Modelling errors are (at least theoretically) knowable.

While Goldstein and Rougier (2009) introduced reified analysis as part of a comprehensive Bayesian framework, we propose to use the concept of a reified model as a useful tool that helps us relate an actual model to the physical system in an attempt to describe conceptual model uncertainty. In essence, we ask the modelling groups to provide three related descriptions a follows:

1) *True System*: Describe in detail current system understanding, including hydrogeological features, processes, and conditions that are considered relevant to understand and predict the behaviour of the bedrock, bentonite, and interface between them.

2) *Reified Model*: Describe a hypothetical model that best represents the true system behaviour, specifically model features that are considered influential.

3) *Actual Model*: Describe in detail the features, processes, and conditions implemented in the actual model used to predict the behaviour of the repository subsystem, including assumptions, simplification, limitations, restrictions and constraints.

4) *Alternative Model*: Describe alternative conceptual models considered viable to explain and predict true system behaviour, or to question or disprove the hypotheses examined with the actual model.

After describing the actual model, the following questions may help arrive at a reified model:

- To what extent would the actual model need to be refined to make it more representative of the true system?
- Which omitted model feature is considered most important for improving model performance (as defined in the task description)?
- If this feature were included in a refined model, what other feature should be considered next for inclusion in an even better model?
- Which alternative conceptual model is a viable candidate to explain the observed system behaviour (or our current understanding thereof), and which alternative explanations can be excluded?
- Which alternative conceptual model is a viable candidate to question or disprove an assumption, hypothesis, or our current understanding?

If no more features in need of improvement can be thought of, one has arrived at the reified model. Note that the term "feature" includes hydrogeologic features, processes, conditions, but also numerical aspects of the model, such as dimensionality, resolution, accuracy of PDE solver, etc.

A2.3 Input and prior uncertainties

Omission, simplifications, and assumptions made during the abstraction and model development process are the source of error and uncertainty in system understanding and model predictions. Before the impact of these assumptions on predictions can be assessed, it is useful to formulate the degree of uncertainty associated with an assumption. This is relatively straight-forward if considering an assumption about a parameter value, which may be uncertain (within bounds) as a result of variability or incomplete knowledge or uncertain characterization data. Assumptions about processes or conditions at the site may be highly uncertain, but difficult to formulate. It is also essential to list features that are omitted from a model, and whose existence in the real system may be very likely.

Note that this step is not concerned with the question of how a model feature affects a prediction (or how uncertainty in the model feature propagates to uncertainty in the model prediction). It is concerned with the state of knowledge about model features that are uncertain or not included in our actual model.

5) *Prior Uncertainties*: Describe and – if possible – quantify the state of knowledge or uncertainty about features that are included or excluded from the actual model.

A2.4 Sensitivities

Conceptual and parametric uncertainties may be acceptable if the corresponding aspect of the model does not significantly influence the overall system understanding or numerical model prediction of interest. The influence of conceptual or parameterized model features on predictions is usually examined by a sensitivity analysis. Most local sensitivity analysis that change one aspect at a time provide useful insights into the system behaviour, but may not include important interactions among features or groups of features, nor do they account for nonlinearities. Nevertheless, many simulations were performed during Task 8, providing quantitative or qualitative insights into the impact of conceptual or parametric inputs on system understanding and model predictions.

6) *Impact on Understanding*: Describe potential impact of model features on overall system understanding.

7) *Impact on Predictions*: Describe and – if possible – quantify impact of model features on specific model predictions.

A2.5 Ranking

It is useful to rank the model features identified during the detailed descriptions of the actual and reified models according to the modeller's belief of their order-of-magnitude impact on model predictions.

8) *Ranking of Features*: If possible, rank model features, omissions, simplifications, and assumptions according to their potential impact on overall system understanding and numerical model predictions.
9) *Weighting of Features*: If possible, assign weights to the ranked model features, omissions, simplifications, and assumptions to reflect the order of magnitude of the expected impact.

A2.6 Prediction uncertainty

Given input uncertainty and sensitivities, the state of knowledge *after* a modelling study (and the associated uncertainty of a model prediction) can be assessed.

10) *Uncertainty in Understanding*: Describe the degree of confidence you have about the overall system understanding given conceptual uncertainties and their impact on that understanding.
11) *Uncertainty in Predictions*: Describe the degree of confidence you have in your model predictions given conceptual uncertainties and their impact on these predictions.

Useful questions to consider include:

- How well do you think a single run of your model represents the true system behaviour?
- What confidence do you have that the true system behaves according to your understanding?
- What would your expectation be if predicting a repeat test in a different tunnel at Äspö, or for a different time scale?
- What confidence do you have that the true system behaviour is within a certain range of your model prediction, and what is this range?
- Which uncertainties are considered aleatoric and thus irreducible?
- Which uncertainties are considered epistemic, and how were they reduced by the selected modelling and analysis approach?

A2.7 Calibration and prediction

Comparisons of model predictions with laboratory and field data may be useful to assess the model's ability to represent the true system (or at least how the true system reveals itself through limited observations, which may in themselves suffer from errors and uncertainties). If adjustments to the conceptual model and its parameters made during calibration are larger than expected, this may indicate that conceptual model uncertainty was underestimated. Moreover, the degree to which model features and estimated parameter values are effective properties rather than representing physical aspects of the true system indicates whether conceptual uncertainties are large and whether the model is suitable for predictive analyses.

12) *Data Uncertainty*: Assess the quality of the BRIE and water-uptake test (WUT) data, i.e. uncertainties and potential systematic errors.
13) *Expected Residuals*: Describe which component of the measured data the model is expected to reproduce and predict (e.g. is it the intent to capture the order-of-magnitude behaviour, average value, general trend, low-frequency fluctuations, high-frequency fluctuations, all details except measurement error, all details including systematic components of measurement errors?).
14) *Prediction*: Describe how well your model predicted the system behaviour observed during the BRIE and WUT experiments.
15) *Calibration*: Describe how well your model reproduced the system behaviour observed during the BRIE and WUT experiments.

The comparison between model prediction and observed data can be described qualitatively, or represented by a quantitative goodness-of-fit measure.

A2.8 Specific predictions

A few performance measures may be used to evaluate the range of predictions as a result of conceptual and parametric uncertainties and for further analyses. We propose that results from Task 8d be used.

16) *Predictions*: Provide the model-predicted best-estimate value of inflow into the open probing holes KO0017G01 and KO0018G01. Provide the model-predicted best-estimate saturations values at the time of dismantling. Provide the model-predicted best-estimate value of the time for bentonite re-saturation to 95 %.
17) *Uncertainty*: Provide the uncertainty (range or distribution) of these predictions based on parametric uncertainties in the actual model used for these predictions. Describe which parametric uncertainties are considered in this assessment.
18) *Conceptual Uncertainty*: Describe the uncertainty of these predictions accounting for conceptual model uncertainties. Describe which conceptual uncertainties are considered in this assessment.

A2.13 General assessment

Task 8 was conducted to gain an improved understanding of a particular repository subsystem. This process of gaining understanding can be thought of as a refinement of the conceptual model of the system; it is associated with a change in our beliefs about how well we understand the system.

19) *Understanding*: Describe the main improvement in system understanding gained by performing Task 8.
20) *Change in Uncertainty*: Describe how uncertainty has changed as new data from BRIE were incorporated into the model.
21) *Conceptual Uncertainty*: Describe the degree to which the current conceptual understanding is believed to represent the behaviour of the true system.
22) *Model Uncertainty*: Describe the degree to which the current numerical model is believed to represent the behaviour of the true system[1].
23) *Key Uncertainty*: Describe which aspect of the conceptual or numerical model is the main source of insufficient system understanding and predictive uncertainty.
24) *Research Plan*: Describe how uncertainty in this main aspect could be reduced by collecting additional information or data, and what specific changes to the actual model could be made to improve system understanding and to reduce predictive uncertainty.

A3 Comparative analysis

A3.1 Goal

The information requested in Chapter 2 (if made available by multiple modelling groups) may be used to summarize the groups overall understanding of this particular repository subsystem. It would also reflect the level of confidence this community has on its understanding of a system it studied by means of conceptual and numerical modelling. By comparing individual assessments and stated confidence in these assessments, an overall, qualitative picture of conceptual uncertainty may be gained. The more quantitative results (requested in Section 2.8) may be evaluated to obtain ranges and statistical measures of uncertainty. They could be further analysed by bootstrapping, concepts of fuzzy logic, cross-verification exercises, and model averaging.

[1] Here we specifically mean the BRIE test setup. You are welcome to consider additional uncertainties relating to deposition holes in a deep repository e.g. thermal processes, but these should be identified under a separate heading to those directly related to the BRIE experiment.

A3.2 Suggested approach

It is intended to elicit the information from the modelling groups via a questionnaire (Table 4-1; attached) and synthesise the responses as follows:

- Collate results and identify consensus and any significant differences between modelling groups.
- Circulate summary to modelling groups prior to Task Force Meeting.
- Present results at Task Force Meeting followed by roundtable discussions to elicit views of the modelling groups regarding:
  - Key assumptions
  - Significant conceptual uncertainties
  - Consensus view of ability to predict bentonite wetting
- Prepare synthesis as a draft paper (plus any supporting material).
- Circulate to modelling groups for revision/comment.
- Revise and submit paper to suitable journal.

This will result in a qualitative evaluation of the uncertainties associated with modelling BRIE. Due to the retrospective nature of the application (lack of true "prior" information) it is not certain that quantitative methods (e.g. Bayesian analyses) can be reasonably applied to the results of the data. For this reason we suggest that before any commitment to quantitative analysis is made, the results from the modelling groups including the questionnaire replies should be reviewed for their ability to support such an assessment.

A suggested timeline for the work is set out below in Table A-1. The aim would be that the questionnaires could be filled in in parallel with reporting by the Modelling Groups to minimise any duplication of effort.

Table A-1. Suggested timeline for comparative analysis.

Early summer 2015	Approach document and draft questionnaire to modelling groups
Task Force Meeting #33 Kalmar	Discussion of approach and any clarifications needed
End 2015	Questionnaire responses back from Modelling Groups (in parallel with report?)
Spring 2016	Collate responses and distribute to Modelling Groups
Task Force Meeting #34	Presentation and roundtable on Uncertainty
Summer 2016	Draft paper circulate for responses
Autumn 2016	Submit revised paper? Possible quantitative analysis

Table A-2. Questionnaire on model uncertainty.

True system, reified model, and actual model		
1	True system	Describe in detail current system understanding, including hydrogeological features, processes, and conditions that are considered relevant to understand and predict the behaviour of the bedrock, bentonite, and interface between them.
2	Reified model	Describe a hypothetical model that best represents the true system behaviour, specifically model features that are considered influential.
3	Actual model	Describe in detail the features, processes, and conditions implemented in the actual model used to predict the behaviour of the repository subsystem, including assumptions, simplification, limitations, restrictions and constraints.
4	Alternative model	Describe alternative conceptual models considered viable to explain and predict true system behavior, or to question or disprove the hypotheses examined with the actual model.
Input and prior uncertainties		
5	Prior uncertainties	Describe and – if possible – quantify the state of knowledge or uncertainty about features that are included or excluded from the actual model.
Sensitivities		
6	Impact on understanding	Describe potential impact of model features on overall system understanding.
7	Impact on predictions	Describe and – if possible – quantify impact of model features on specific model predictions.
Ranking		
8	Ranking of features	If possible, rank model features, omissions, simplifications, and assumptions according to their potential impact on overall system understanding and numerical model predictions.
9	Weighting of features	If possible, assign weights to the ranked model features, omissions, simplifications, and assumptions to reflect the order of magnitude of the expected impact.
Prediction uncertainty		
10	Uncertainty in understanding	Describe the degree of confidence you have about the overall system understanding given conceptual uncertainties and their impact on that understanding.
11	Uncertainty in predictions	Describe the degree of confidence you have in your model predictions given conceptual uncertainties and their impact on these predictions.
Calibration and prediction		
12	Data uncertainty	Assess the quality of the BRIE and water-uptake test (WUT) data, i.e. uncertainties and potential systematic errors.
13	Expected residuals	Describe which component of the measured data the model is expected to reproduce and predict (e.g. order-of-magnitude behaviour, average value, general trend, low-frequency fluctuations, high-frequency fluctuations, all details except measurement error, all details including systematic component of measurement error).
14	Prediction	Describe how well your model predicted the system behaviour observed during the BRIE and WUT experiments.
15	Calibration	Describe how well your model reproduced the system behaviour observed during the BRIE and WUT experiments.
Specific predictions		
16	Predictions	Provide the model-predicted best-estimate value of inflow into the open probing holes KO0017G01 and KO0018G01. Provide the model-predicted best-estimate saturation values at the time of dismantling. Provide the model-predicted best-estimate values of the time for bentonite re-saturation to 95 %.
17	Uncertainty	Provide the uncertainty (range or distribution) of these predictions based on parametric uncertainties in the actual model used for these predictions. Describe which parametric uncertainties are considered in this assessment.
18	Conceptual uncertainty	Describe the uncertainty of these predictions accounting for conceptual model uncertainties. Describe which conceptual uncertainties are considered in this assessment.
General assessment		
19	Understanding	Describe the main improvement in system understanding gained by performing Task 8.
20	Change in uncertainty	Describe how uncertainty has changed as new data from BRIE were incorporated into the model.
21	Conceptual uncertainty	Describe the degree to which the current conceptual understanding is believed to represent the behaviour of the true system.
22	Model uncertainty	Describe the degree to which the current numerical model is believed to represent the behaviour of the true system.
23	Key uncertainty	Describe which aspect of the conceptual or numerical model is the main source of insufficient system understanding and predictive uncertainty.
24	Research plan	Describe how uncertainty in this main aspect could be reduced by collecting additional information or data, and what specific changes to the actual model could be made to improve system understanding and to reduce predictive uncertainty.

Appendix B

Scientific publications resulting from Task 8

Dessirier B, 2016. Numerical modeling of groundwater and air flow between compacted bentonite and fractured crystalline rock. PhD thesis. Stockholm University.

Dessirier B, Jarsjö J, Frampton A, 2014. Modeling two-phase flow interactions across a bentonite clay and fractured rock interface. Nuclear Technology 187, 147–157.

Dessirier B, Frampton A, Jarsjö J, 2015. A global sensitivity analysis of two-phase flow between fractured crystalline rock and bentonite with application to spent nuclear fuel disposal. Journal of Contaminant Hydrology 182, 25–35.

Dessirier B, Frampton A, Fransson Å, Jarsjö J, 2016. Modeling early in situ wetting of a compacted bentonite buffer installed in low permeable crystalline bedrock. Water Resources Research 52, 6207–6221.

Dessirier B, Åkesson M, Lanyon B, Framton A, Jarsjö J, 2017. Reconstruction of the water content at an interface between compacted bentonite blocks and fractured crystalline bedrock. Applied Clay Science 142, 145–152.

Finsterle S, Lanyon B, Åkesson M, Baxter S, Bergström M, Bockgård N, Dershowitz W, Dessirier B, Frampton A, Fransson Å, Gens A, Gylling B, Hančilová I, Holton D, Jarsjö J, Kim J-S, Kröhn K-P, Malmberg D, Pulkkanen V-M, Sawada A, Sjöland A, Svensson U, VidstrandP, Viswanathan H, 2018. Conceptual uncertainties in modelling the interaction between engineered and natural barriers of nuclear waste repositories in crystalline rock. In Norris S, Neeft E A C, Van Geet M (eds). Multiple Roles of Clays in Radioactive Waste Confinement, Geological Society, London, Special Publications 482. doi:10.1144/SP482.12

Hančilová I, Hokr M, 2016. Coupled hydro-mechanical model of bentonite hydration and swelling. IOP Conference Series: Earth and Environmental Science 44.

Hančilová I, Hokr, M, Novák, J, 2017. Bentonite saturation from discrete fractures – numerical model of non-uniform swelling over a gap. Procedia Engineering 191, 530–535.

Kröhn K-P, 2012. Qualifying a computer program for simulating fracture flow. Computing and Visualization in Science 15, 29–37.

Kröhn K-P, 2017. Characterising groundwater flow in the fractured rock at Äspö, Sweden. Computing and Visualization in Science 2017, 185–192.

Appendix C

Glossary

Background rock	Modelling term referring to geologic material other than discretely implemented *large fractures* or *intermediate fractures*; typically represented by an effective continuum.
Bedrock	Geologic environment, specifically the fractured granitic rock near the BRIE site.
Feature	General term for a geologic or hydrogeologic structure, engineered structure, or distinctive attribute of a model.
Host rock	Geologic environment hosting a planned or actual nuclear waste repository.
Intermediate fracture	Fractures larger than *small fractures* and smaller than *large fractures*; typically stochastically included in DFN model.
Large fracture/feature	Large fractures that are discretely, deterministically included in numerical model; may be deformation zone or fracture zone consisting of multiple fractures.
Probing hole	76-mm diameter vertical holes drilled into the floor of the BRIE test bed; used for initial characterisation and selection of location for *surrogate deposition holes.*
Rock mass	Modelling term referring to geologic material between the fractures that are explicitly implemented in discrete fracture network (DFN) model; includes solid, intact *rock matrix* and all fractures that are not explicitly included in the DFN model, i.e. micro-fractures and *small fractures.*
Rock matrix, matrix	Solid, intact, unfractured rock.
Small fracture	Fractures smaller than the mapping cut-off length.
Surrogate deposition hole	300-mm diameter vertical holes in the floor of the BRIE test bed; generated by widening *probing holes*; filled with bentonite buffer to simulate deposition hole conditions; used to study bentonite-rock interactions, specifically water inflow for bentonite hydration.

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