

International Collaborations on Engineered Barrier Systems: Brief Overview of SKB-EBS Activities

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SUMMARY

Research collaborations with international partners on the behavior and performance of engineered barrier systems (EBS) are an important aspect of the DOE-NE Used Fuel Disposition Campaign strategy in the evaluation of disposal design concepts. These international partnerships are a cost-effective way of engaging in key R&D activities with common goals resulting in effective scientific knowledge exchanges thus enhancing existing and future research programs in the USA. This report provides a brief description of the activities covered by the Swedish Nuclear Fuel and Waste Management Company (SKB) EBS Task Force (TF) (referred hereafter as SKB EBS TF) and potential future directions for engagement of the DOE-NE UFDC program in relevant R&D activities. Emphasis is given to SKB EBS TF activities that are still ongoing and aligned to the UFDC R&D program. This include utilization of data collected in the bentonite rock interaction experiment (BRIE) and data sets from benchmark experiments produced by the chemistry or “C” part of the SKB EBS TF. Potential applications of information generated by this program include comparisons/tests between model and data (e.g., reactive diffusion), development and implementation of coupled-process models (e.g., HM), and code/model benchmarking.

ACRONYMS

BBM	Basic Barcelona Model
BRIE	Bentonite Rock Interaction Experiment
CIEMAT	Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas
CEC	Cation Exchange Capacity
CI	Cement – Opalinus Clay Interaction (Mt. Terri URL)
DFT	Density Functional Theory
DOE	Department of Energy
EBS	Engineered Barrier System
HRL	Hard Rock Laboratory (Äspö site)
HM	Hydrological Mechanical
LBNL	Lawrence Berkeley National Laboratory
MD	Molecular Dynamics
NBS	Natural Barrier System
NE	Nuclear Energy
OPA	Opalinus Clay Rock (Mt. Terri URL)
R&D	Research and Development
SKB	Swedish Nuclear Fuel and Waste Management Company
SNL	Sandia National Laboratories
TF	Task Force
THM	Thermal-Hydrological-Mechanical
THMC	Thermal-Hydrological-Mechanical-Chemical
UFD	Office of Used Fuel Disposition Research and Development
UFDC	Used Fuel Disposition Campaign
URL	Underground Research Laboratory

1. INTRODUCTION

The SKB Engineered Barrier System (EBS) Task Force (referred hereafter as the SKB EBS TF) is a consortium of international participants conducting R&D work related to EBS activities at the Äspö Hard Rock Laboratory (HRL). This is part of the much broader SKB Task Force that also includes activities related to modeling of Groundwater Flow and Transport of Solutes (GWFTS). These activities will not be covered in this part of the report since the focus is on those associated with buffer/backfill interactions and chemical issues in the near-field environment. There are nine tasks in the SKB TF (see Table 1) in which tasks 1 through 8 are either completed or approaching near completion. Task 9 was proposed recently with the goal of developing more realistic models to represent solute transport and retardation in the natural rock matrix. More details of these SKB TF activities can be found at <http://www.skb.se/taskforce/modelling-tasks/>. The DOE-NE recently joined this task force as part of the international collaborations activities within the Used Fuel Disposition Campaign (UFDC).

Table 1. Summary of modeling tasks for the SKB TF.

Task	Brief Description	Status
1	Long-term (pumping, dilution, tracer) test experiments, evaluation, modeling	Completed
2	Äspö field tracer experiments; small-scale (1 - 10 m) design calculations/modeling	Completed
3	The Äspö tunnel experiment; predictive/evaluation modeling of site scale tunnel excavation	Completed
4	Tracer Retention and Understanding Experiments (TRUE); Predictive modeling of tracer test experiments	Completed
5	Integration of hydrogeology and hydrochemistry; assess impact of Äspö tunnel construction on groundwater	Completed
6	Performance assessment (PA) modelling using site characterization (SC) data (PASC)	Completed
7	Reduction of performance assessment (PA) uncertainty through site scale modeling of long-term pumping at the Olkiluoto site, Finland	Completed
8	Bentonite Rock Interaction Experiment (BRIE) - Interaction between engineered and natural barriers	Nearing Completion
9	Develop models that in a more realistic way represent solute transport and retardation in the natural rock matrix	Currently Proposed

2. OBJECTIVE

The objective of the SKB EBS TF is the “development of general and effective tools for the advanced coupled THMC analysis of buffer and backfill behavior” (SKB EBS TF documentation). This goal of this task force is to support long-term efforts to assess the prediction thermal-hydrological-mechanical (THM) evolution of the clay-bearing backfill/buffer and its interactions with EBS components (e.g., canister and rock).

The main THM objectives are:

- Verify the capability to model THM processes in unsaturated and saturated bentonite buffer / backfill materials.
- Validate and further develop material models and computer simulation tools by numerical THM modeling of laboratory and field tests. Validation and testing are achieved by comparisons between modeling and experimental measurements.
- Evaluate the influence of parameter variations, parameter uncertainties, and model imperfections.

THM-related tasks within the SKB EBS TF include: prototype repository, homogenization, sensitivity analysis, and Bentonite Rock Interaction Experiment (BRIE). These activities are related to task 8 and are expected to be finalized soon. However, data generated from these activities can be used in model testing and validation. Extensive descriptions of these activities can be found in project documentation and in the scientific literature. However, a brief description of each THM activity is given in the following sections. Successively, a description of the chemistry issues within SKB EBS TF is given with emphasis on buffer/backfill interactions.

2.1 Prototype Repository

The prototype repository is a study to construct a full-scale representation (KBS-3 type) of the planned deep geological repository for Swedish spent nuclear fuel (Lydmark, 2011). The project was conducted at the Äspö Hard Rock Laboratory (HRL) within crystalline rock at approximately 450 meters deep (Figure 1). The layout of the prototype repository consists of six vertical deposition holes spatially arranged in two sections (see Figure 2 relative to main tunnel access). Each deposition hole contains an electrically heated canister backfilled with bentonite. The deposition holes are instrumented with (*in situ*) sensors and fluid sample collectors.

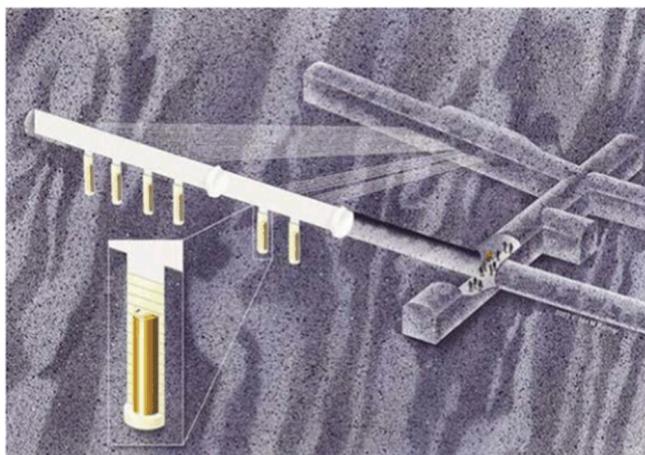


Figure 1. Schematic figure showing deposition holes and tunnel layout for the prototype repository (Andersson et al. 2005 - EC document).

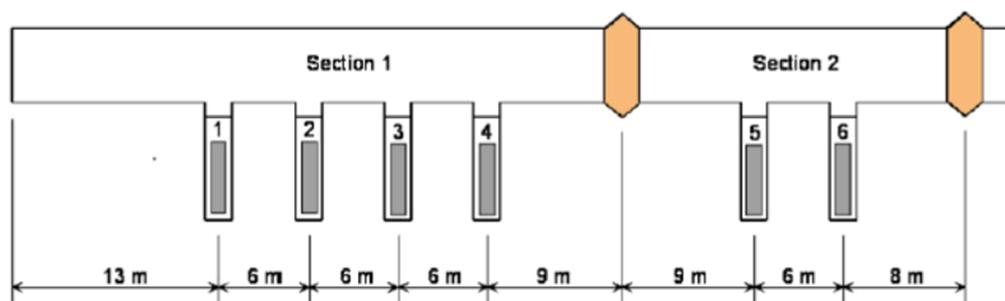


Figure 2. Cross-sectional view of the prototype repository showing deposition holes and their spacing (Lydmark, 2011).

Field characterization of the site hydrological features of the site were conducted through boreholes cored in the vicinity of the testing area for monitoring and sample collection (e.g., water inflow, chemical/microbial conditions). Some of the relevant goals for this sampling cover monitoring and characterization of chemical/microbial activity, effects of temperature on water-rock interactions, model testing, and clay buffer redox chemistry (Lydmark 2011). Modeling activities of the obtained data are planned to continue supporting the development of the envisioned THM model. The usage of dismantling data has been proposed in this activity.

2.2 Clay Buffer Homogenization

The goal of clay buffer homogenization experiments is to improve our understanding of hydro-mechanical (HM) phenomena of clay swelling under saturated conditions. The existence of gaps and holes in bentonite can lead to heterogeneities in the emplaced buffer/backfill clay material. Such heterogeneities can impact the bulk transport properties of the backfill and thus the isolation performance of the EBS. Therefore, these experiments are important to evaluate the fate of buffer/backfill upon hydration and the capacity for effective self-sealing and water saturation in the presence of these heterogeneities. Moreover, the data generated in these studies are key to the development and validation/verification of HM models aimed at representing this process. The experiments consist of small- and large-scale tests evaluating radial swelling and buffer homogenization, respectively.

The small-scale radial swelling tests are designed to assess one-dimensional axial swelling, swelling and closure of an axisymmetric outer space, and swelling and closure of an axisymmetric inner hole (see Figure 3). The large-scale experiments consist of a cylinder having dimensions of 300 mm in diameter and a height of 100 mm (Figures 4a and 4b). A central cylindrical device is placed at the center to mimic the presence of a waste canister. A bentonite (MX-80) block (ring geometry) is mounted inside the cylinder that is tightly enclosed with a lid. The device is fitted with pressure transducers to measure swelling pressure and suction. Water is inserted around the radial surface and through inlet cavities. The test is conducted at near saturation until the bentonite is completely homogenized. Modeling efforts of these experiments are ongoing with proposed extension of this approach to unsaturated conditions.

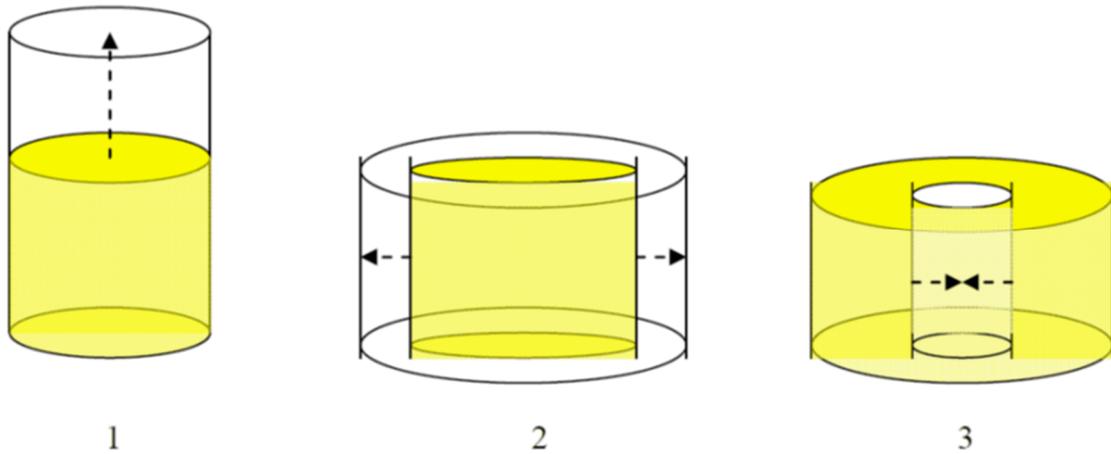


Figure 3. (1) One-dimensional axial swelling in a cylindrical space; (2) swelling and closure of an axisymmetric and concentric outer space; and (3) swelling and closure of an axisymmetric and concentric inner hole. (Source: SKB EBS TF documentation).

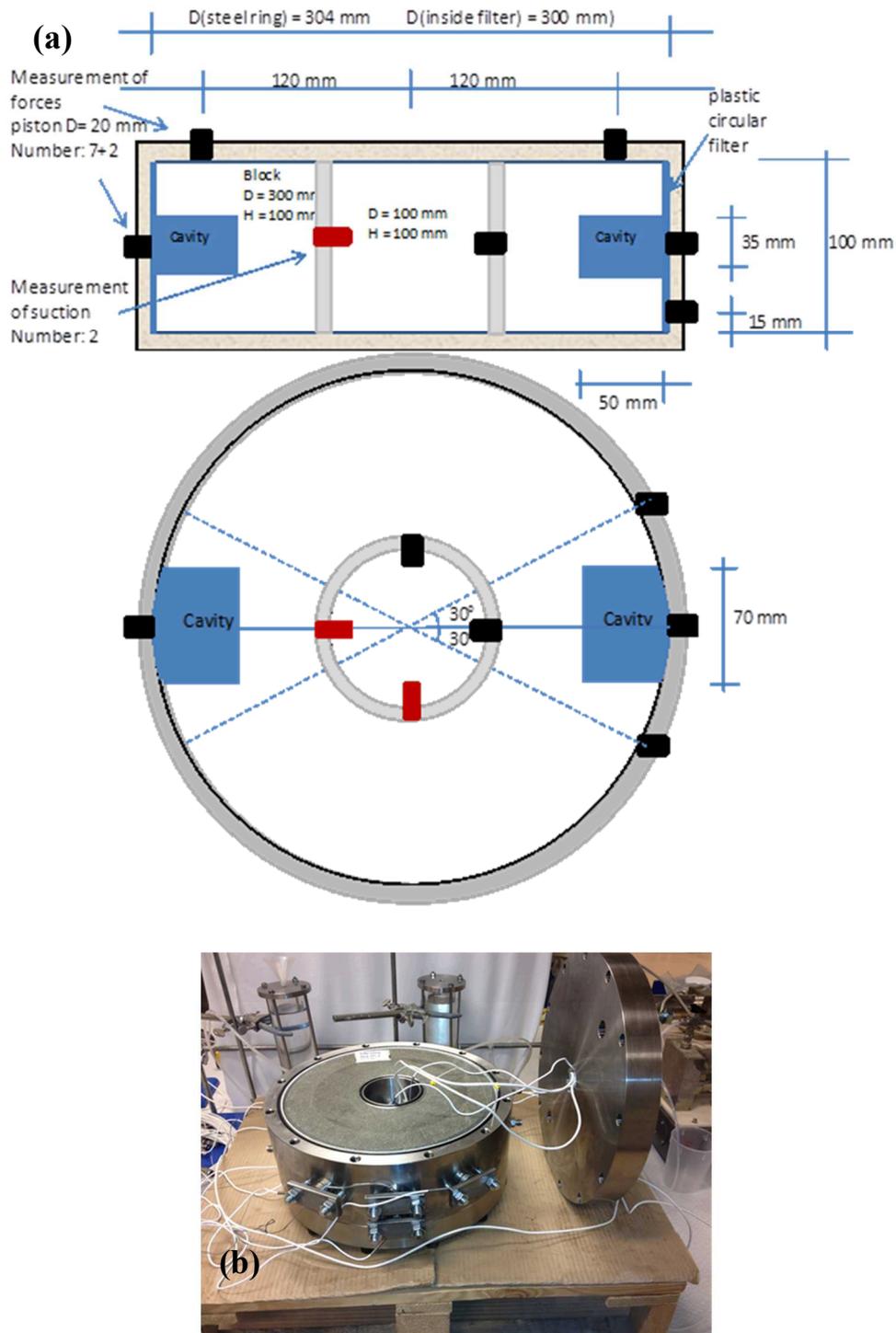


Figure 4. Schematic view of device geometry used in the large-scale buffer homogenization experiments (a). Photo of device showing lid, inlets, and sensor instrumentation along with bentonite block. Source: Börjesson et al. (2016).

2.3 Sensitivity Analysis

The main objective of this activity is to evaluate the effects of parameter uncertainties on the results of EBS process model simulations (Schäfers, 2010). The expectation is that this analysis should advance the following:

- Improve the understanding of coupled-processes relevant to EBS.
- Identify and rank key parameters in coupled-process models.
- Code validation/verification (benchmarking).

The latter can be represented by code inter-comparison for a matrix of EBS processes that include THM, vapor diffusion, and temperature-dependent fluid density and viscosity. Code inter-comparisons activity evaluating these processes were conducted for a 2D axisymmetric geometry representing a KBS-3V deposition hole with a heated canister backfilled with bentonite and surrounded by crystalline rock. The results of this modeling exercise were presented by Dr. Annika Schäfers at the SKB TF meeting held at the Lawrence Berkeley National Laboratory (LBNL) on December 2014. The current focus is on code validation/verification exercises although sensitivity analysis is a topic it's still pursued.

2.4 Bentonite Rock Interaction Experiment (BRIE)

The main goal of the Bentonite Rock Interaction Experiment (BRIE) is to yield experimental data obtained at the Äspö Hard Rock Laboratory to support modeling efforts (<http://www.skb.se/taskforce/modelling-tasks>). The experiment consists of vertical deposition boreholes in crystalline rock filled with unsaturated bentonite. The deposition boreholes were drilled in regions of the host rock having both few fractures with different transmissivity and no fractures at all. The emplaced bentonite was instrumented for monitoring of total stress, pore water pressure, and RH. The bentonite parcels were subsequently over-cored and analyzed for water content distribution. The main goals in these experiments are (Fransson et al. 2014):

- Gain enhanced knowledge of the exchange of water across the bentonite-rock interface.
- Characterization of water flow in rock matrix and fractures.
- Improve our knowledge of bentonite wetting to advance model predictions. This includes characterization of water pressure, bentonite clay swelling pressure, and water content.

Figures 5 and 6 show the dimensions of bentonite parcels and sample locations, respectively. Figure 7 shows water retention data collected *in situ* in the form of water content vs. relative humidity (RH) in the bentonite.

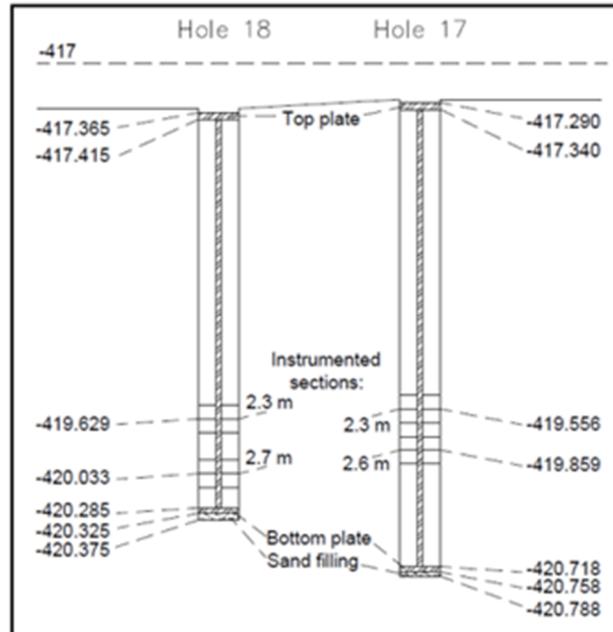


Figure 5. Schematic diagram showing the dimensions of deposition boreholes 17 and 18. Source: Fransson et al. (2014).

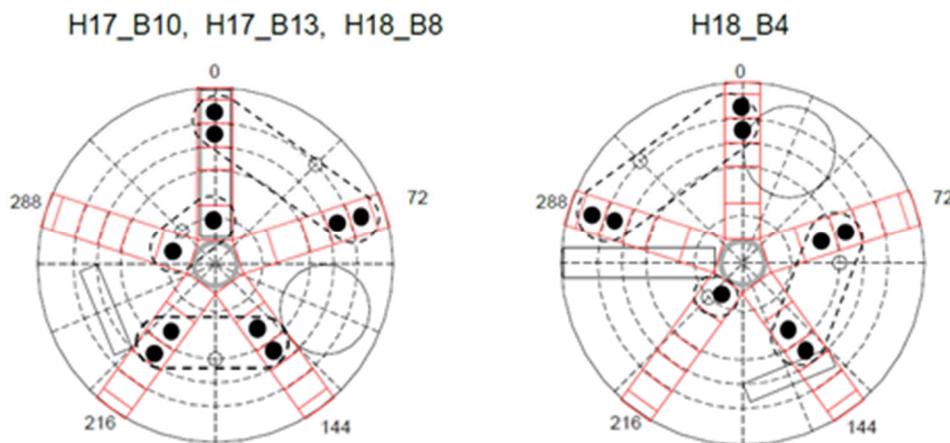


Figure 6. Schematic figure of deposition holes showing a flat view of sample locations (filled circles) and RH sensors (open circles). Source: Fransson et al. (2014).

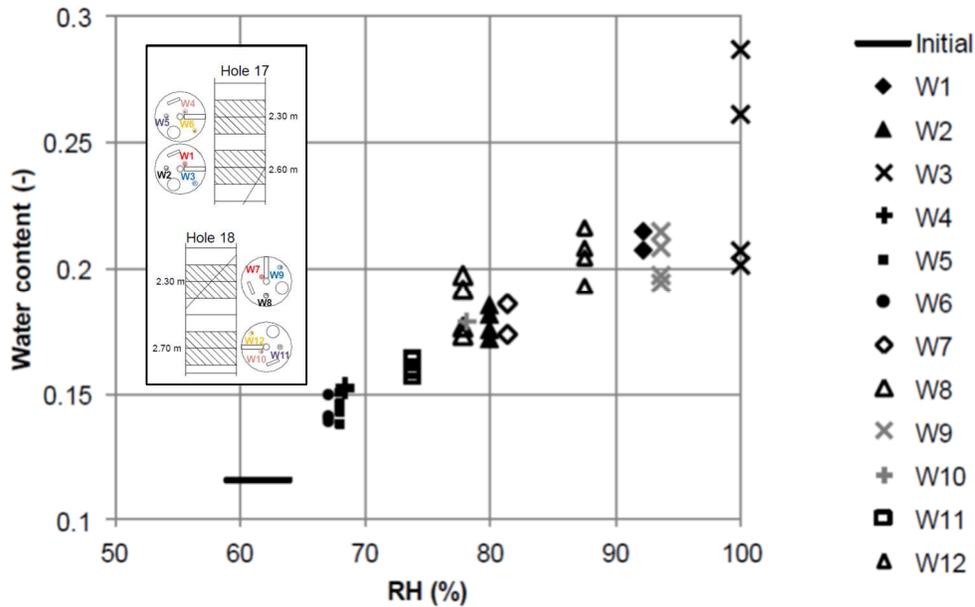


Figure 7. Water retention data as function of RH. Inset shows sensor locations in deposition holes. Source: Fransson et al. (2014).

2.4.1 Clay Hydration Modeling: Model/Data Comparisons

An initial comparison was made between a thermodynamic model developed for smectite hydration against a microporosity model based on bentonite hydration data. The water retention data from the BRIE experiment shown in **Figure 7** were used here for comparison. Details of the thermodynamic model adopted for smectite hydration implemented in the Cantera code is described in Jové Colón et al. (2013). One of the goals of this thermodynamic model is to capture the effect of smectite composition on clay hydration using a sub-regular Margules-type solid solution formulation. This thermodynamic model is calibrated using water adsorption/desorption data on unconfined smectites with different cation components (Na, Ca, K, and Mg).

The microporosity model advanced by Sedighi and Thomas (2014) is based on a more simplified Margules clay solid solution representation advanced by Ransom and Helgeson (1994) for water uptake by the smectite clay interlayer. Distinctions are made through the model formulation between macroporosity and microporosity. In this model, microporosity refers to the saturated smectite interlayer porosity largely responsible for clay swelling. Macroporosity is represented by the pore space between clay grains and aggregates which is dependent on clay density. This model hinges on the assumption that the volumetric water content of the clay interlayer equals its microporosity assuming full saturation and defined as (Sedighi and Thomas, 2014):

$$n_{micro} = X_{hs} \frac{n_c v_{il}}{Fw_{sm}} \rho_{dry}^{sm}$$

n_{micro} is the microporosity, X_{hs} denotes the mole fraction of hydrated smectite, Fw_{sm} signifies the formula weight of anhydrous smectite, n_c stands for the number of waters in the interlayer,

v_{il} delineates the molar volume of water in the interlayer, and ρ_{dry}^{sm} refers to the smectite dry density. Sedighi and Thomas (2014) calibrate this formulation clay hydration data for MX-80 and FEBEX bentonites. Although both models have a thermodynamic basis, the one by Jové Colón et al. (2013) is built on a consistent set of standard thermodynamic properties of the clay solid and liquid phases. The latter is mainly calibrated to water retention data for bentonites. It should be noted that the thermodynamic model described in Jové Colón et al. (2013) is calibrated on water adsorption/desorption data for exchanged montmorillonite phases with nominally end-member composition. These data is of course different from that adopted by Sedighi and Thomas (2014) for bentonite hydration in their model calibration.

The above formulation used by Sedighi and Thomas (2014) seems advantageous due to its simplicity and ease of implementation. However, there are certain key assumptions like the assumed number of water in the interlayer along with the calibration of X_{hs} to clay hydration data. The parameter X_{hs} can be rather non-linear due to variable clay hydration behavior according to clay structure and composition. Also, the parameter n_c can vary among different studies. For example, Sedighi and Thomas (2014) adopted an n_c value of 4.5 after the work of Ransom and Helgeson (1994) whereas Jové Colón et al. (2013) used a value of 5.5. Still, comparisons between model and data can be made to exemplify the effects of clay composition on hydration behavior. Figures 8 and 9 show the relation between RH and X_{hs} from three bentonite hydration studies (FEBEX, MX-80, and BRIE). The model/data given by Sedighi and Thomas (2014) has been corrected for n_c equals 5.5 for a valid comparison with the thermodynamic model described in Jové Colón et al. (2013). Similarly, retrieval of the parameter X_{hs} from the SKB BRIE water content data (Fransson et al., 2014) was computed assuming a n_c value of 5.5. The microporosity model shown in Figure 8 is calibrated to Na-smectite (powder) and compacted bentonite MX-80. This model trends appears to represent the data satisfactorily although with some deviations (Figure 9), even within the scatter of the experimental data. Similarly, the thermodynamic model for Na-smectite provides a reasonable representation of the data trend for bentonite MX-80 and BRIE with some deviations as well. The differences in the two model trends advanced by Sedighi and Thomas (2014) are described by differences in sample state: powder for Na-smectite and compacted bentonite MX-80. The authors asserted that the compacted bentonite MX-80 trend provides a better representation of the experimental data. However, the hydration behavior dependence on the state of the clay sample (compacted versus powder) is still a subject of research.

As expected, both models exhibit strong dependencies on data calibration but particularly on clay composition. The thermodynamic model (Jové Colón et al., 2013) is calibrated from adsorption/desorption data of nominally end-member montmorillonite clay compositions. The predicted clay hydration curves by the thermodynamic model illustrate distinctive trends between monovalent and divalent cationic smectite compositions. Sedighi and Thomas (2014) observed a comparable behavior between MX-80 and FEBEX bentonites – the authors described the latter as predominantly having a mixed Ca-Mg smectite component. Therefore, clay hydration will be strongly influenced by its mineral structure and composition. Both modeling approaches appear to provide reasonable bounds for the clay compositional effect. The explicit thermodynamic treatment of clay and fluid in the Cantera implementation along with data consistency can bring advantages when extending the model to problems involving geochemical interactions. However, its implementation with coupled hydrological-mechanical (HM)

simulations schemes as a robust constitutive model can be quite involved. More work is needed in the comparison of clay hydration data from multiple sources and various barrier clay materials.

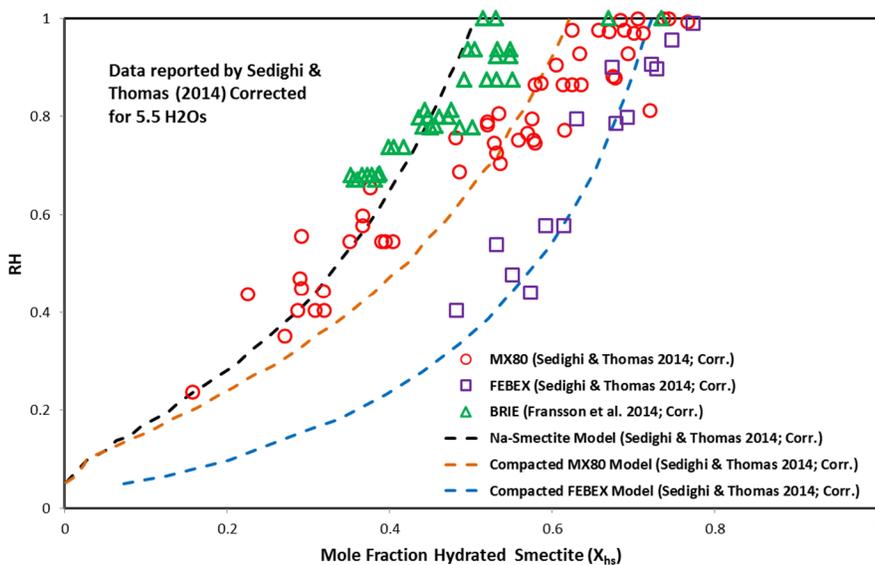


Figure 8. Plot of RH vs. X_{hs} for bentonite hydration in URL experiments and the model predictions of Sedighi and Thomas (2014). The BRIE experimental data is consistent with MX-80 bentonite. Data/model of Sedighi and Thomas (2014) is corrected for X_{hs} assuming n_c equals 5.5 for comparison with the thermodynamic model described in Jové Colón et al. (2013).

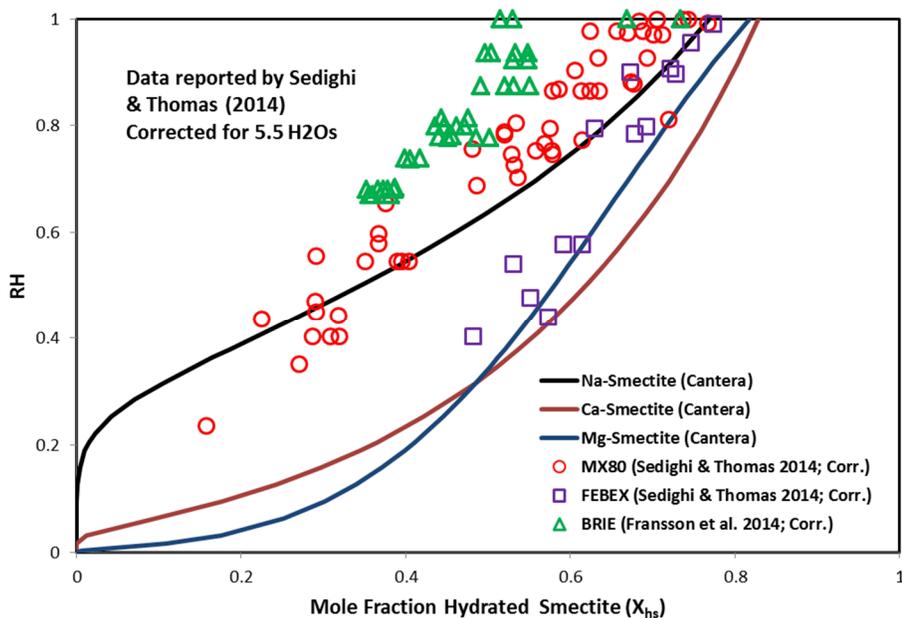


Figure 9. Plot of RH vs. X_{hs} for bentonite hydration in URL experiments and the model predictions of Jové Colón et al. (2013) for Na, Ca, and Mg smectite. The BRIE experimental data is consistent with MX-80 bentonite. Data/model corrected for X_{hs} assuming n_c equals 5.5 for comparison with the thermodynamic model described in Jové Colón et al. (2013).

3. SKB EBS Task Force – Chemical Issues

The part on chemical issues or commonly referred as “C” within the SKB EBS TF began in 2006 with the objective of developing tools to analyze THMC couplings in the evaluation of buffer and backfill behavior. As a result of a discussion at the EBS TF meeting in Barcelona in 2015, the following points describe the main focus outlined by in a SKB TF internal communication by Dr. Urs Mäder (University of Bern, May 2015):

- “To develop and test alternate porosity concepts that explain fundamental properties like ion and water transport and swelling pressure
- To assemble experimental data sets (literature and/or own experiments) that allow testing of alternate concepts and assess so their relative merits
- To gain insight at the molecular scale of physico-chemical processes within smectite interlayers (e.g., via MD simulations)
- To further develop numerical tools that allow for a general implementation of these chemical aspects into a THM framework.”

The above points represent key fundamental issues to the safety assessment given their influence to EBS performance. The scientific assessment of these items includes both experimental and modeling efforts where chemical phenomena need to be part of the coupled-process system of THM issues. Although limited resources to make advancements in both experimental and modeling work has been recognized, some achievements have been made by either members of the task force or by others. As a result, a set of benchmarks has been defined to generate the necessary data to address issues such as reactive diffusion in clay and the nature of porosity in these systems.

3.1 Experimental Benchmarks for Modeling

Currently there are five benchmark data sets in the SKB EBS TF generated by experiments aimed to capture various levels of complexity of reactive transport in clay. These include variability in aqueous solution and clay chemistry, effects of secondary phases, reactive diffusion, and ion exchange phenomena.

3.1.1 Benchmark 1: Salt Diffusion in Montmorillonite

This benchmark experiment evaluates diffusion of salts through (Na/Ca) montmorillonite clay. To effectively prevent ion exchange, the cation type of the source saline solution is equal to the charge-compensating cation in the montmorillonite structure. **Figure 10** shows the experimental setup used in this experiment (Birgersson, 2011). The experimental device is fitted with a pressure transducer to measure swelling pressure. Various source solution compositions were considered:

- 1 M, 0.4 M and 0.1 M NaCl in the Na-montmorillonite case.
- 0.4 M, 0.1 M, and 0.25 M CaCl₂ in the Ca-montmorillonite case.

The target solution was maintained diluted during the experiment. Electrochemical measurements were used to measure electrolyte concentrations in the target solution. The key measurements in this experiment are the swelling pressure (axial stress) and salt concentration in the target solution. Also, measurements of water/solid mass ratio were performed upon tests by weight difference between dry and wet samples. Experimental data for this experimental is

available through the SKB EBS TF website. This type of experiments are discussed in Birgersson et al. (2009).

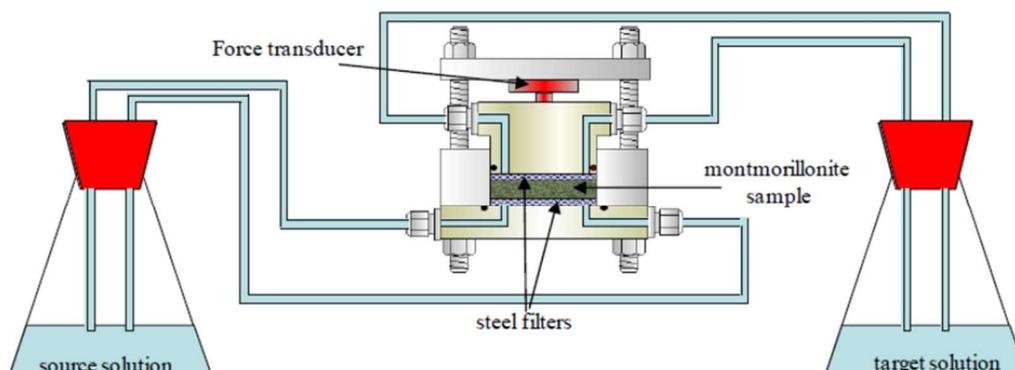


Figure 10. Experimental setup for benchmark 1 involving salt diffusion experiment in montmorillonite (Birgersson, 2011; Birgersson et al., 2009).

3.1.2 Benchmark 2: Gypsum Dissolution in Na- and Ca-Montmorillonite

This benchmark experiment is similar to benchmark 1 since the experimental setup is the same but the clay sample is different. This experiment evaluates through-diffusion and gypsum dissolution in a mixed sample of montmorillonite clay and gypsum in a configuration depicted in **Figure 11**. Gypsum powder is sandwiched between water-saturated montmorillonite clay samples. Water saturation was attained by monitoring the stabilization of swelling pressure in the cell. Experiments and data collection were conducted in the same fashion as in benchmark 1. Through-diffusion and gypsum dissolution experiments were performed by controlled solution concentrations in the source and target solution reservoirs. This allows for control of chemical gradients induced by solution concentration in the reservoirs. The experiments were conducted in configurations of Na-montmorillonite – Gypsum – Na-montmorillonite and Ca-montmorillonite – Gypsum – Ca-montmorillonite. These experiments are important in evaluating the potential effects of secondary minerals in bentonite. Such effects have been identified in bentonite hydrothermal experiments (Cheshire et al., 2014) where degradation of secondary phases could yield marked effects on the altered mineral assemblage and solution chemistry.

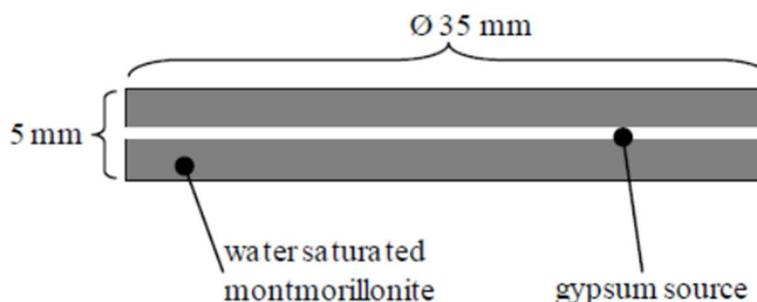


Figure 11. Sample configuration for benchmark 2 experiments (Birgersson, 2011).

3.1.3 Benchmark 3: Ca/Na Ion Exchange in Montmorillonite

This benchmark consists of ion exchange experiments on compacted Na-Ca montmorillonite having different densities and test solutions (Birgersson, 2011). These experiments are also discussed in Birgersson et al. (2009). The purpose of these tests is to evaluate ion exchange equilibria along with diffusion of Na and Ca in saturated montmorillonite clay. It also investigates the effects of solution chemistry on swelling pressure. The experimental cell shown in Figure 12 is similar to benchmarks 1 and 2 except that input solutions are recirculated through the semi-permeable membrane filters (Birgersson, 2011). Swelling pressure was monitored constantly to confirm the attainment of an equilibrium state. Chemical analyses of different equilibrium states were used in the evaluation of cation exchange capacity (CEC).

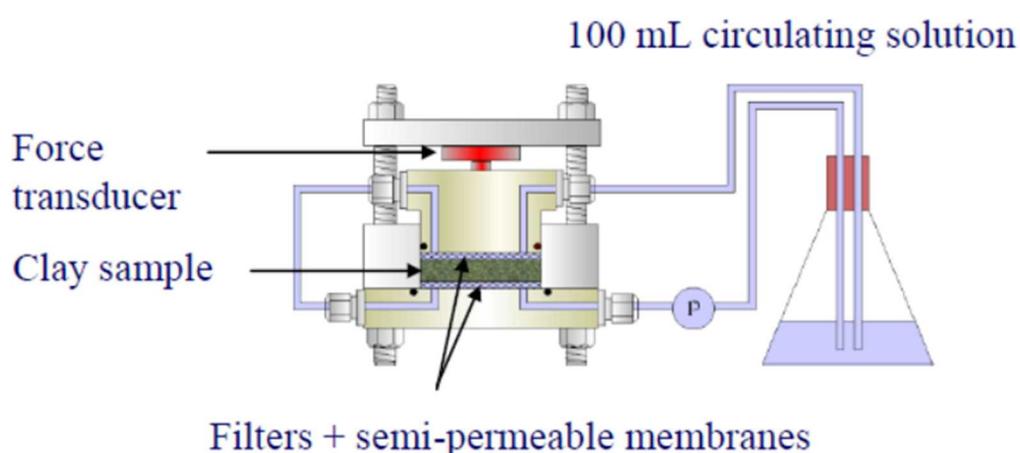


Figure 12. Experimental setup for benchmark 3 to investigate ion exchange and effect on swelling pressure (Birgersson, 2011; Birgersson et al., 2009).

3.1.4 Benchmark 4: Multi-Component Advective-Diffusive Transport Experiment in MX-80 Compacted Bentonite

Benchmark 4 investigates a percolation experiment (Figure 11) where an input solution of synthetic groundwater is injected through a sample of bentonite MX-80 (Birgersson, 2011). The pressure difference (i.e., hydraulic gradient) in the sample is maintained constant throughout the experiment while keeping constant flow. This allows for periodic sampling of outlet solutions with time. The setup also allows for monitoring of hydraulic and electrical conductivity. Experimental data consisting of solution concentrations of synthetic groundwater constituents (Na^+ , K^+ , Mg^{++} , Ca^{++} , Sr^{++} , Cl^- , Br^- , SO_4^- , NO_3^- , and deuterium) are available the SKB EBS TF website. Alt-Epping et al. (2015) provides reactive transport simulations for four computer codes using this benchmark. These authors also examine the effects of electrostatic effects on diffusion using the appropriate implementation in the simulation code. Such benchmarking exercise is not only important for code inter-comparisons but also to evaluate the significance of capturing pore-scale versus continuum effects (upscaling). This allows for analyzing the adequacy or predictive capability of reactive-transport model implementations and their use in the PA of a repository.

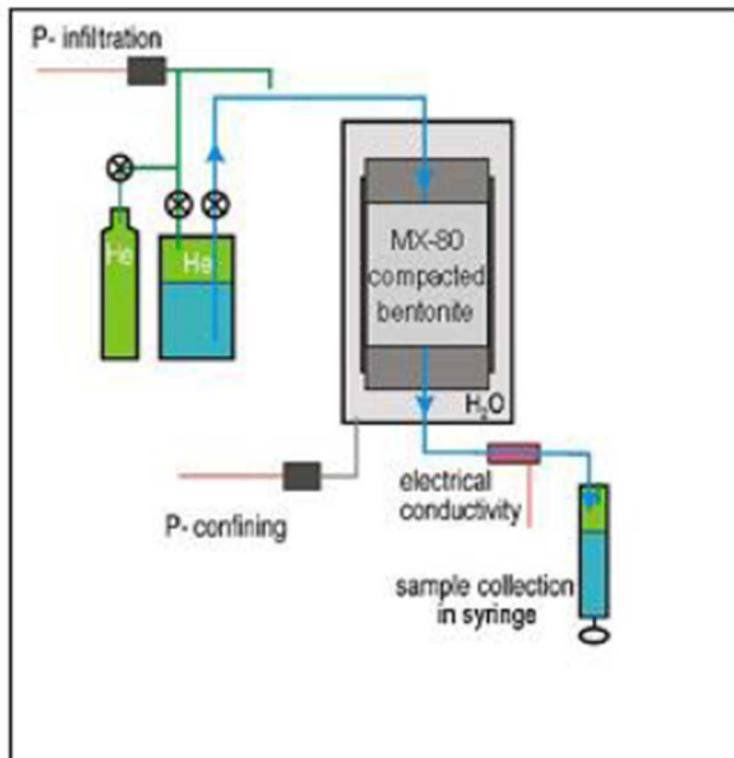


Figure 11. Schematic diagram of percolation experiment setup for compacted bentonite (Birgersson, 2011).

3.1.5 Benchmark 5: Diffusion of Selected Anions through Compacted Bentonite

This benchmark describes the diffusion of the anions Cl^- , I^- , and SeO_4^{2-} in compacted Czech bentonite (Birgersson, 2011; Hofmanová and Červinka, 2014). Radionuclides of these anionic species ($^{36}\text{Cl}^-$, $^{129}\text{I}^-$, and $^{79}\text{SeO}_4^{2-}$) were used in the diffusion experiments. The aim of this study is to evaluate anionic retardation due to electrostatic effects in saturated bentonite at constant ionic strength of 0.1 M. The experimental setup is made up of a diffusion cell (Figure 12) containing compacted bentonite between two solution reservoirs (source and target). The bentonite sample is lined at each fluid contacting face with stainless steel filters. Samples were saturated under vacuum conditions.

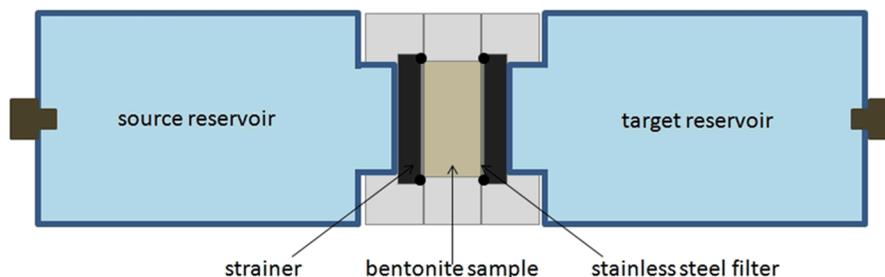


Figure 12. Schematic diagram showing diffusion cell used in benchmark 5 (Birgersson, 2011; Hofmanová and Červinka, 2014).

4. FY16 and Future Outlook

There is still continuing work within Task 8 targeting existing and future modeling activities. Some of the data generated in this task could be used in test cases (e.g., clay hydration modeling in a previous section) or in future model development. The focus on future SKB EBS TF chemical issues and ongoing work in benchmarks (1 – 5) provide a varied platform of collaboration tasks that are aligned with UFDC experimental and modeling activities, for example:

- Molecular dynamics (MD) and first principles modeling of clay interlayer chemistry – MD modeling has been identified as a potential future activity in the SKB EBS TF part on chemical issues. This work could target sorption dynamics at clay edge sites and diffusion effects using the expertise from the UFDC R&D on MD modeling on clay. Another potential activity is the application of density functional theory (DFT) simulations to evaluate the dynamics of clay dehydroxylation on montmorillonite. Dehydroxylation phenomena at interlayers can potentially exert key chemo-mechanical effects on the interlayer chemistry.
- Diffusion in compacted clay (model/experiment) – Experimental and modeling activities on diffusion through clay conducted at LBNL and LLNL can benefit from similar work in the SKB EBS TF (benchmarks 1 – 5). This collaboration should be centered on the leveraging of existing data to examine the effects of electrostatics on reactive diffusion in porous clay.
- The effect of soluble or unstable phases in the buffer/backfill clay matrix – Current UFDC experimental activities on clay interactions have revealed the effects of minor phases on the high temperature degradation of barrier clay material (Cheshire et al., 2014). Benchmark 2 has provided a data set on the effect of gypsum dissolution embedded with clay under ambient conditions.

The above R&D activities have common goals for potential collaboration with the DOE UFDC. No decision has been made yet on what particular activity to join or delineation of specific goals. Such details need to be agreed upon by all interested parties to then make decisions on any future R&D target and task engagements.

5. References

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