The illustration in the lower right of Figure 3-67 shows the location of LTDE-SD in the Äspö HRL tunnel system. In the center of the figure, the local tunnel section is depicted together with the different boreholes drilled from the site. These boreholes include the LTDE-SD borehole and the closely located pilot borehole. These two boreholes intersect a water-conducting natural fracture at a distance of 11 m from the tunnel wall, which is the experiment's target fracture. The LTDE-SD borehole was drilled with different diameters, roughly described as follows. Up to the fracture plane the borehole has a large diameter and beyond the fracture plane a small diameter was used. This is simplistically illustrated in the lower left of Figure 3-67. The borehole is indicated by the solid black line and the intersected fracture is indicated by the curved blue line. Orange areas indicate packed-off volumes, whereas blue areas indicate volumes of the tracer cocktail. The red arrows symbolize in-diffusion of tracers from the large-diameter borehole through the fracture surface and into the underlying altered rock matrix. They also symbolize diffusion into the unaltered rock matrix from the small-diameter borehole. The dashed black line indicates the rock volume that was overcored at the end of the tracer test.

The tracers injected were Na-22, S-35, Cl-36, Co-57, Ni-63, Se-75, Sr-85, Nb-95, Zr-95, Tc-99, Pd-102, Cd-109, Ag-110, Sn-113, Ba-133, Cs-137, Gd-153, Hf-175, Ra-226, Pa-233, U-236, and Np-237. Tracer concentrations as well as other environmental parameters were monitored during the 200 days the tracer test progressed. After that the surrounding rock volume was overcored, and from the overcored volume a number of smaller drill cores were excavated, as illustrated on the left in Figure 3-68. Here the natural fracture surface is located on the right-hand side of the overcored rock volume. A large number of the core samples of Figure 3-68 were cut into subsamples as indicated to the right in Figure 3-68, enabling the obtaining of tracer penetration profiles. Tracer concentrations (or activities) in the rock were obtained by a number of analysis methods, including autoradiography on intact samples; direct activity measurements on intact and crush samples; and leaching or dissolution of intact and crush samples, followed by water phase measurements.

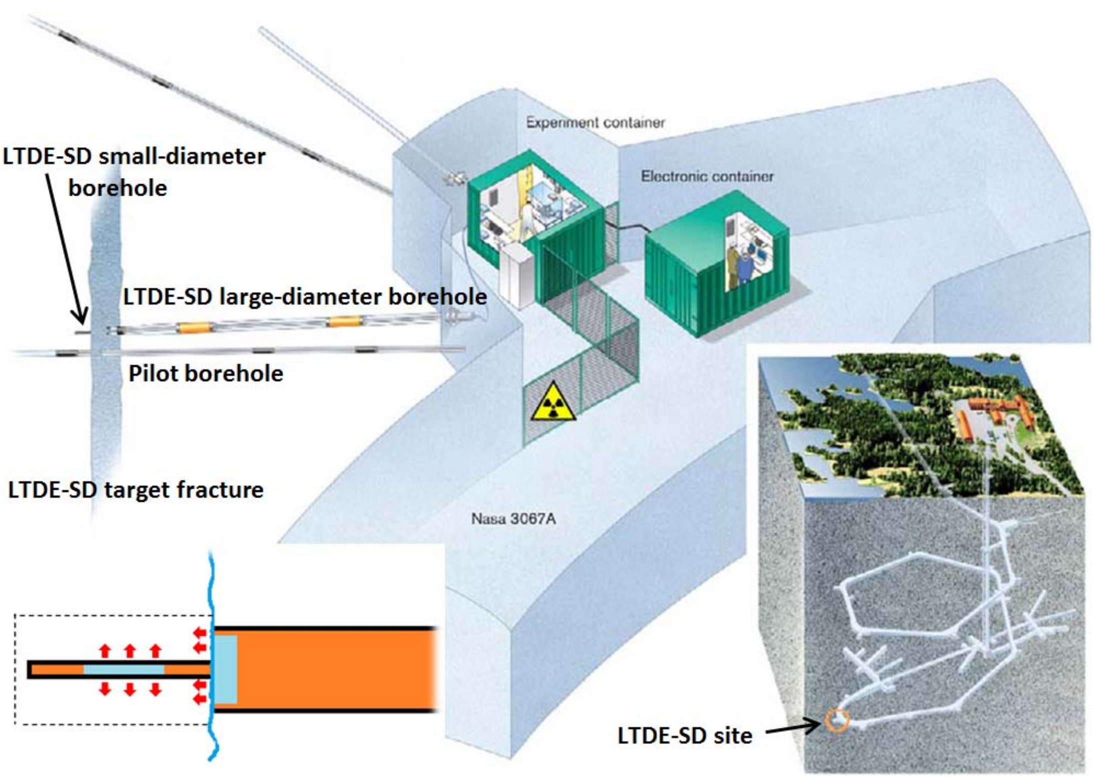


Figure 3-67. Schematic layout of LTDE-SD at Äspö HRL (from SKB, 2011a)

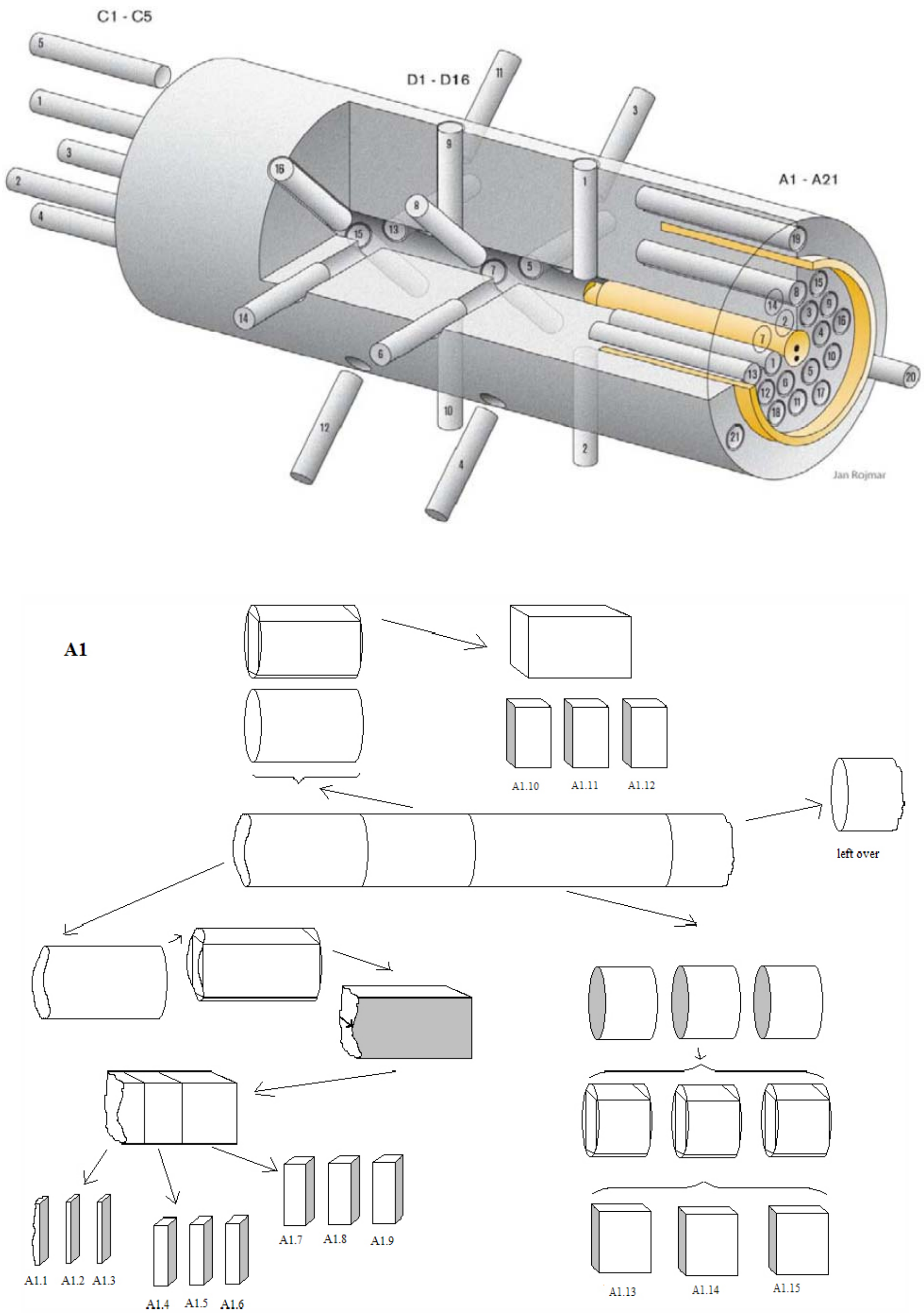


Figure 3-68. Illustration of the sampling of the overcored rock volume in LTDE-SD (from SKB, 2011a)

Results from the overcoring rock volume in LTDE-SD provide concentration profiles in the rock matrix that are not fully understood to date. Figure 3-69 shows experimental concentration profiles of two tracers compared to predictive model results, with obvious discrepancies in the curve shapes. These may be a result of heterogeneities in the rock matrix or may be related to inappropriate model assumptions related to Fickian diffusion or equilibrium sorption. One aim of Task 9 will be to increase realism in the diffusion-sorption predictions of the LTDE-SD.

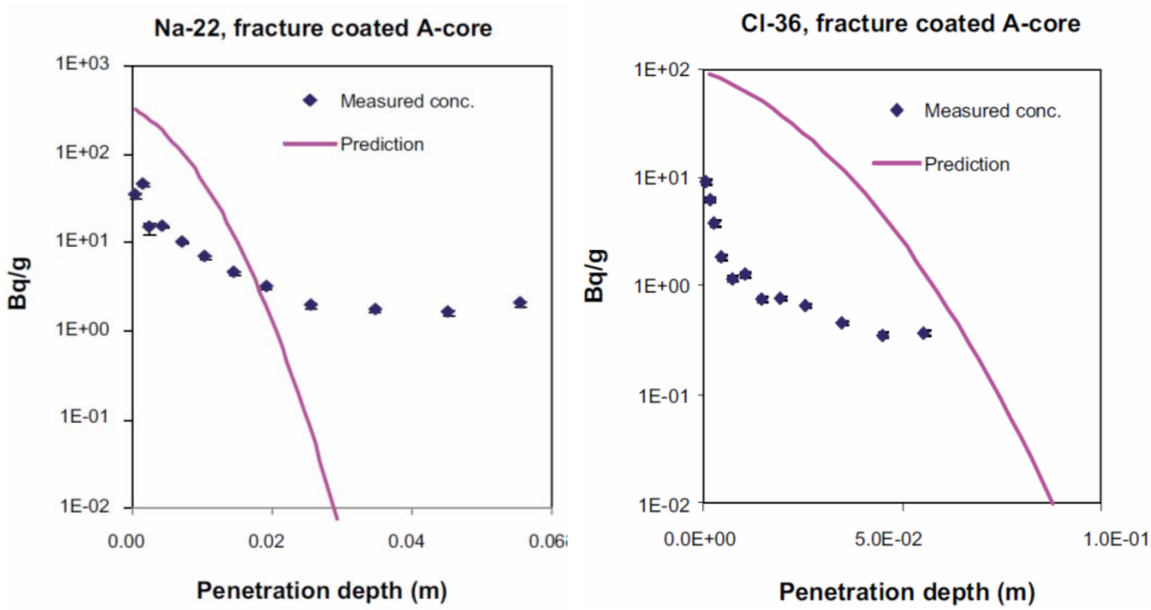


Figure 3-69. Results from the in-situ in-diffusion experiment LTDE-SD through a natural fracture surface. Modeled Na-22 and Cl-36 penetration profiles (solid curves) are compared to the measured profiles (diamonds). Na-22 activities in the rock matrix were obtained on intact of crushed rock slices and Cl-36 activities were obtained by leaching of intact or crushed slices.

The REPRO experiments are the other important element of Task 9. REPCO involves a number of boreholes that have been drilled into the non-fractured rock matrix from a working niche at the Onkalo underground rock characterization facility, at about 400 m depth (see Figure 3-70). Borehole ONK-PP323 is utilized for the Water Phase Diffusion (WPDE) series of experiments, which are advection-diffusion-sorption tests. They are carried out between ~18-20 m from the tunnel wall. A 1.9 m long section has been packed off, and in this section a dummy has been placed. Its diameter is 54 mm whereas the borehole diameter is 56 mm, leaving a 1 mm gap between the borehole wall and the dummy. This gap is regarded as an artificial fracture of relatively well-defined geometry. A very low steady state water flow has been applied in this gap, directed towards the tunnel. This is achieved by injecting the water at the far end of the packed-off section, as shown to the upper right in Figure 3-70. In this water flow the tracers HTO, Na-22, Cl-36, and I-125 were injected in WPDE-1, and HTO, Na-22, Cl-36, Sr-85 and Ba-133 in WPDE-2. Injection was made as a few hours long pulse at the far end of the experimental section. As the pulse travels with the water flow, its tracers diffuse into the rock matrix. As the pulse passes, the concentration gradients are reversed and the tracers diffuse out of the rock matrix and into the flowing water. To date, two experiments have been performed at different flow rates; WPDE-1 (20 µL/min) and WPDE-2 (10 µL/min). The tracer concentrations were measured in water flowing out of the experimental section, both by on-line Na(Tl)I-scintillation detection and by analyzing water samples in the laboratory. Breakthrough curves have been obtained over half a year and about one and a half a year for WPDE-1 and WPDE-2, respectively. Currently there are no plans for overcoring of the rock volume surrounding the experimental section.

Another REPRO experiment, referred to as Through Diffusion Experiment (TDE), will be carried out between three parallel boreholes situated perpendicular to each other, in 1 m long packed-off sections, at a distance of about 11 to 12 m from the tunnel wall. Borehole ONK-PP326 will be used as the injection hole and boreholes ONK-PP324 and ONK-PP327 as observation holes (see Figure 3-70, upper left corner). The distances between the boreholes are between 10 and 15 cm. Advective flow between the boreholes is foreseen to be insignificant, as the experiment takes placed in a rock volume that lacks in water-bearing fractures. The tracers HTO, Na-22, Cl-36, Ba-133, and probably Cs-134 are planned to be injected. The decreasing and (expected) increasing tracer concentrations in the injection hole and observations holes, respectively, will be analyzed. This is done on extracted samples in the laboratory, by liquid scintillation counting and High Resolution x-ray spectroscopy (gamma measurements). Furthermore, on-line measurements will be performed in the injection hole and observation holes by a High Performance Germanium detector and a Na(Tl)I-scintillation detector, respectively. Tracer concentrations in the injection hole will be measured at a higher frequency at the first part of the experiment, while focus will be shifted towards analyzing breakthrough concentrations in the observation holes as the experiment progresses. Breakthroughs of non-sorbing tracers are foreseen within the timeframe of conducting Task 9, although unexpectedly low pore diffusivities may prevent this from happening. The tracers were chosen to make overcoring and analysis of tracer penetration profiles possible, although this option is presently not included in the REPRO planning. As the REPRO project is ongoing, it offers the possibility of both inverse and predictive modeling. The in-situ part of REPRO aims to tackle the topics of diffusion, sorption, anion exclusion, and rock matrix anisotropy. The laboratory part has, in addition, focused on small-scale rock characterization. This provides a wealth of input data that can be incorporated in the modeling.

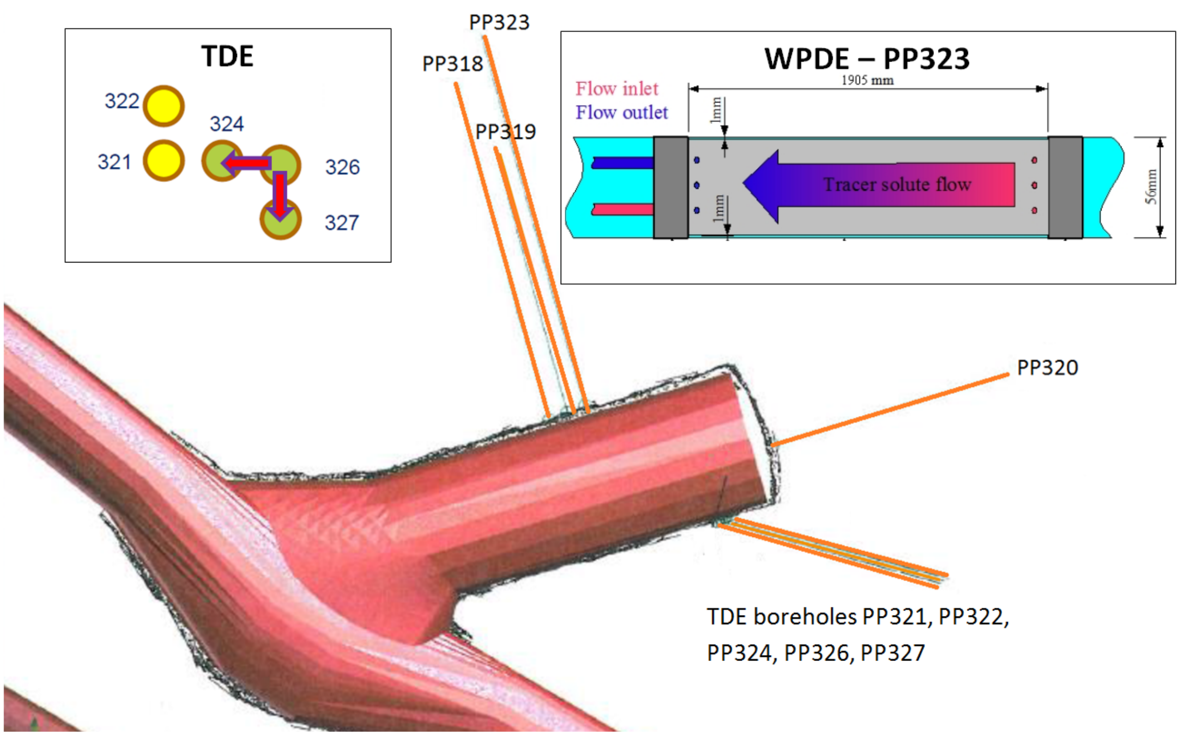


Figure 3-70. The REPRO Niche at the 401 m level at ONKALO, and the nine boreholes drilled from the niche. Borehole PP323 is utilized for WPDE-1&2, and boreholes PP324, PP326, and PP327 for TDE.

3.4.3 EBS-THM Task Force

As mentioned above, the EBS Task Force essentially has two distinct focus areas, one on THM processes referred to as EBS-THM (led by Antonio Gens from UPC in Spain), the other on chemical processes referred to as EBS-C (led by Urs Maeder of University of Bern). The main objective of the EBS-THM Task Force is the development and application of general and effective tools for the advanced coupled THMC analysis of buffer and backfill materials, and their interactions with a saturated fractured host rock environment. Specific goals are as follows: (1) to verify the capability to model THM processes in unsaturated as well as saturated bentonite buffer and backfill materials, (2) to validate and further develop material models and computer codes by numerical THM modeling of laboratory and field tests and compare modeling results with measured results, and (3) to evaluate the influence of parameter variations, parameter uncertainties and model imperfections. There are three ongoing modeling tasks in the EBS-THM task force, all of which have been running for several years and are expected to wind down in 2016 or 2017: the Homogenization Task, the Prototype Repository, and the BRIE experiment which is shared with the GWFTS Task Force (see Section 3.4.2.1). The Homogenization Task and the Prototype Repository Task are briefly described below, followed by a review of possible future tasks in the EBS-THM Task Force.

3.4.3.1 Homogenization Task

SKB has been undertaking an experimental program with a series of laboratory experiments to better understand and quantify homogenization of bentonite backfill. Gaps and cracks may exist due to initial bentonite emplacement or due to long-term hydraulic and chemical erosion of bentonite (the latter refers the possibility of low-ionic strength waters affecting bentonite). 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.

The Homogenization Task is a modeling task supporting the experimental program. Modeling teams developed predictive models for bentonite homogenization, which were then being tested in comparison to results from the experimental series. Figure 3-71 shows a typical experimental setup for a laboratory experiment as part of the Homogenization Task. This experiment was designed to investigate the swelling and potential self-sealing of an irregular cavity that was deliberately cut into a bentonite block in two diametrical positions as shown in the figure. Because these experiments involved the study of saturated bentonite, water for hydration was provided along the radial surfaces and in the cavities. Nine transducers for measuring swelling pressure and two for measuring suction were installed as shown in Figure 3-71. Experimental results showed that complete homogenization of the bentonite block incorporating the two cavities occurred after about 4 months, a result that then needs to be explained by the simulation models. UFD researchers are not currently active in this task.

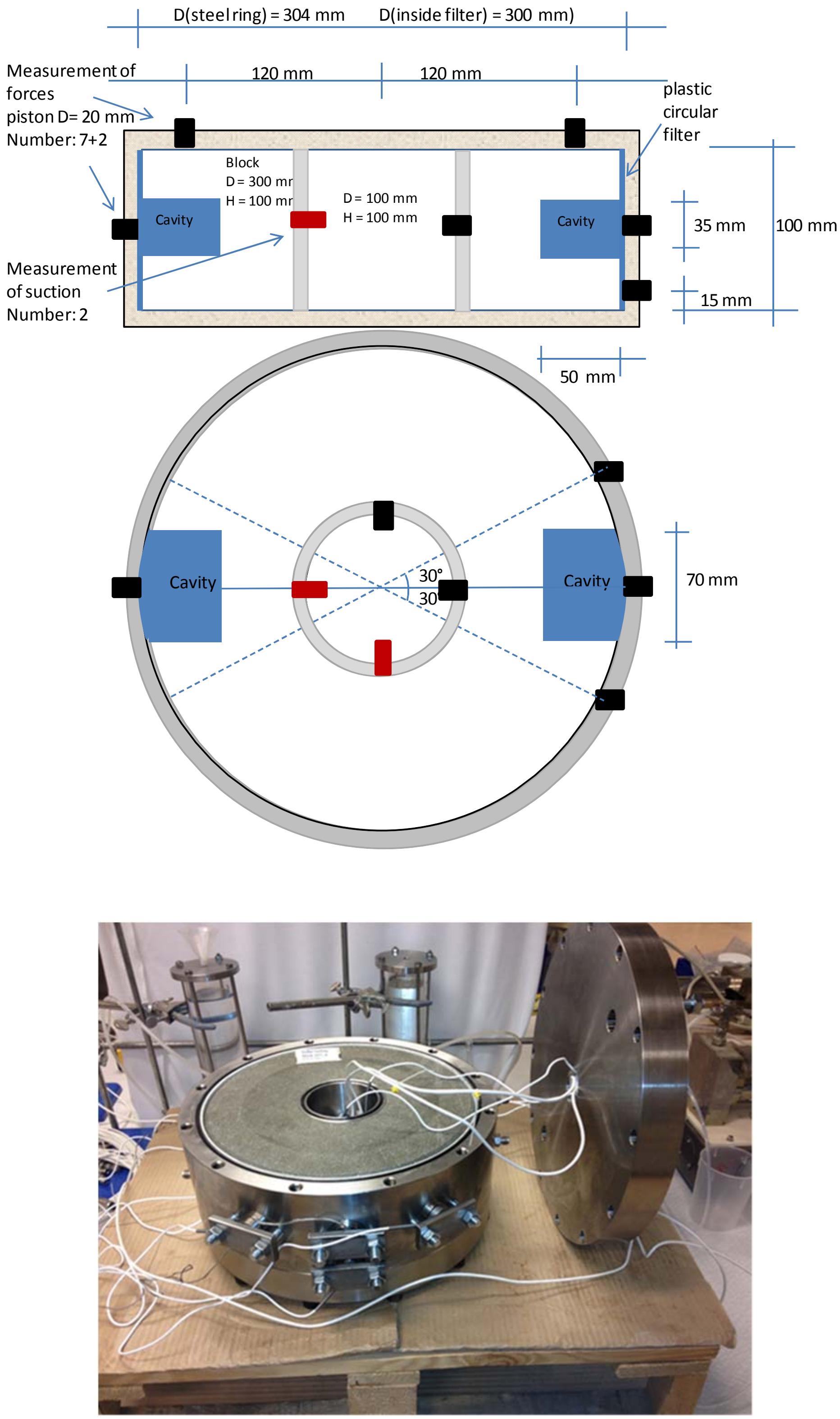


Figure 3-71. Top: Schematic view of device geometry used in the large-scale buffer homogenization experiments. Bottom: Photo of the device showing the lid, inlets, and sensors along with bentonite block (from Börgesson et al., 2015)

3.4.3.2 Prototype Repository

In 2000, SKB started the planning and installation of a so-called Prototype Repository as a full-scale demonstration of the integrated function of the repository, and a reference for testing predictive models concerning individual components as well as the complete repository system. The test area is located in the innermost section of the TBM tunnel at Äspö HRL. The layout involves a total of six deposition holes, four in an inner and two in an outer section—see Figure 3-72. Canisters with dimension and weight according to the current plans for the final repository, and with heaters to simulate the thermal energy output from the spent nuclear fuel, have been positioned in the holes and surrounded by bentonite buffer. The deposition holes were placed with a center distance of 6 m. This distance was evaluated considering the thermal diffusivity of the rock mass and the maximum acceptable temperature of the buffer. The deposition tunnel was backfilled with a mixture of bentonite and crushed rock (30/70). A massive concrete plug, designed to withstand full water and swelling pressures, separates the test area from the open tunnel system, and a second plug separates the two sections. This layout provides two more or less independent test sections. The monitoring system is comprised of a dense network of sensors for temperature, total pressure, pore-water pressure, relative humidity and resistivity, as well as some rock mechanical measurements. The heaters of the inner section were turned on in 2001; those in the outer section in 2004. This was followed by several years of monitoring, offering a very valuable data set of early-stage, full-scale repository evolution.

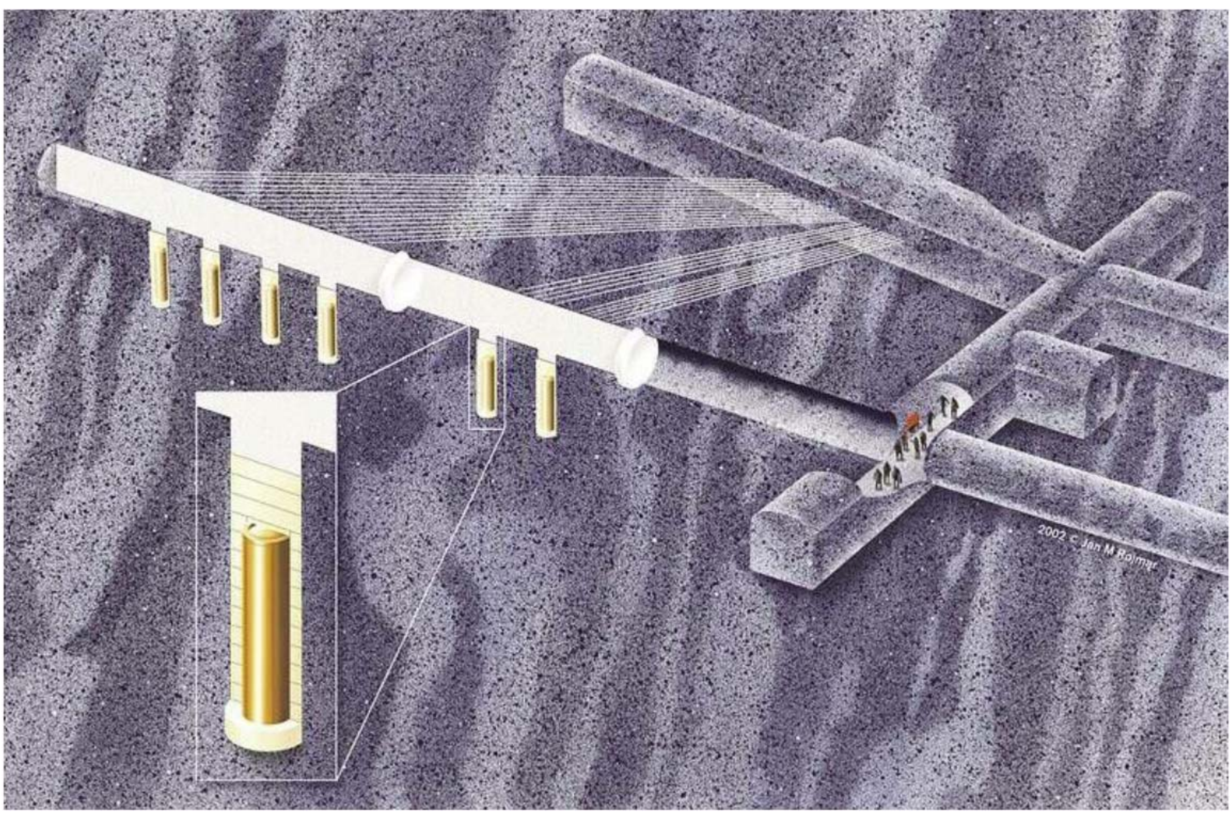


Figure 3-72. Schematic layout of Prototype Repository at Äspö HRL (from SKB, 2011a, 2011b)

In 2011, SKB excavated the outer section of the Prototype Repository while extensive samplings were performed. Approximately 1,000 samples of the backfill and about 3,000 samples of the buffer were taken to determine water content and density. The two canisters were lifted up and transported to SKB's

Canister Laboratory in Oskarshamn for additional investigations. The main objectives of dismantling the outer section were to (1) investigate the density and water saturation of the buffer and backfill, (2) investigate the interface between buffer – backfill and between backfill – rock surfaces, after 7 years of wetting, (3) measure and examine the canisters (positions, mechanical stress, corrosion), (4) investigate the bedrock after dismantling, (5) study biological and chemical activities in the buffer and backfill, and (6) study possible changes of the buffer material caused by temperature and saturation processes. The observations made in one of the excavated deposition holes (Figure 3-73) are the focus of the prototype Repository modeling task of the EBS Task Force, the objective being to verify the THM processes occurring during heating and resaturation, and validation against the post-mortem analysis. The task involves modeling of one of the two outer deposition holes. UFD researchers are not currently participating in this task.

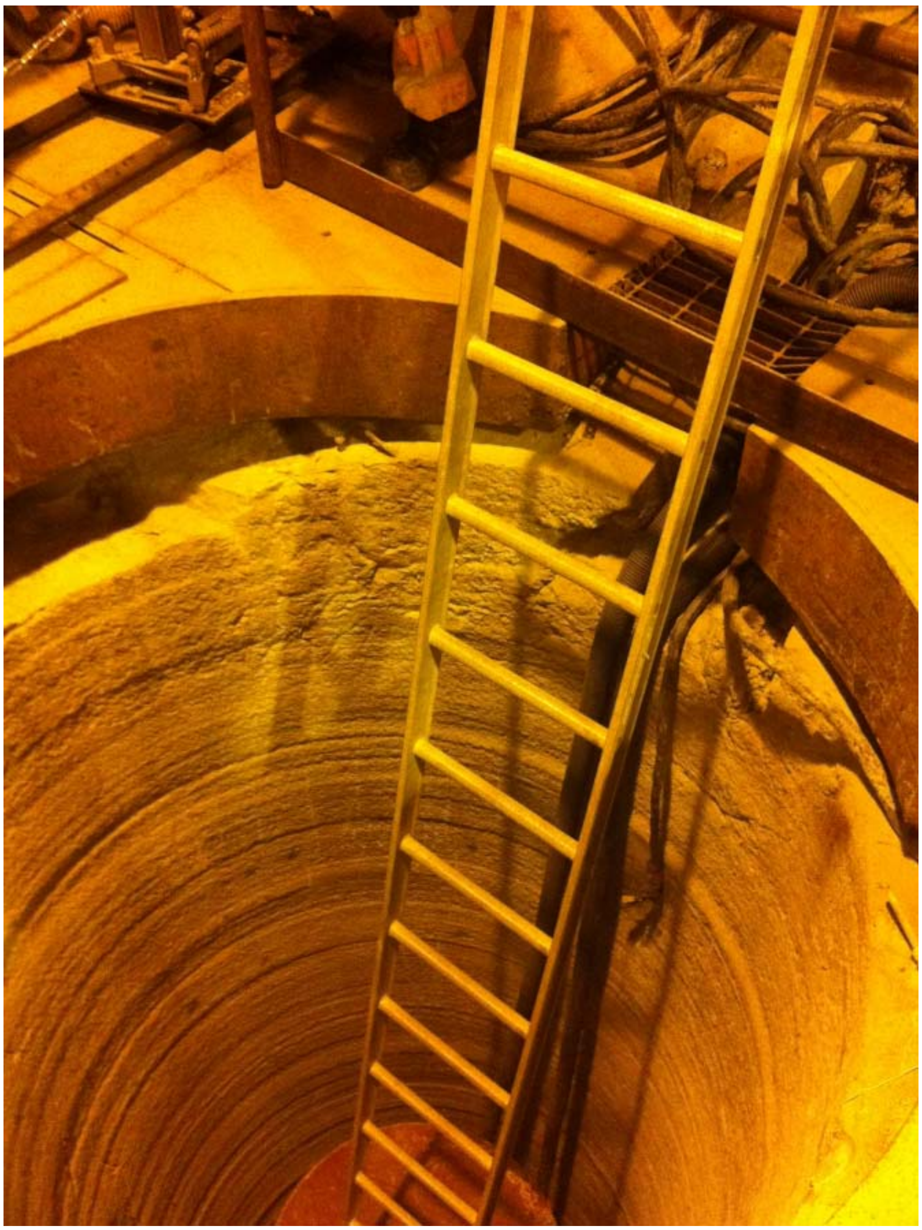


Figure 3-73. Prototype Repository at Äspö HRL: Photo of excavated deposition hole

3.4.3.3 Potential Future EBS-THM Tasks and Outlook

The EBS-THM Task Force is considering initiation of new tasks and has been soliciting input from its task force participants. Several ideas have been brought up in recent meetings in Berkeley (December 2014) and Barcelona (May 2015), some of which may be of relevance to DOE/UFD:

- Task on homogenization in unsaturated barriers (as a continuation of the Homogenization task described in Section 3.4.3.1)
- Task on modeling of water transport in pellet filled laboratory chambers, which would aim to develop new material models for the time-dependent water uptake simulations of pelletized buffer materials
- Task on modeling the FEBEX-DP Experiment (see details in Section 3.3.2)
- Task on gas transport in bentonite utilizing new gas injection laboratory experiments conducted by the University of Bern

The above R&D activities have common goals for potential collaboration with the DOE UFD. However, no decisions on future task selection have been made to date. DOE/UFD will be represented at future task force meetings and will help finalize the future task list of the EBS-THM Task Force.

3.4.4 EBS-C Task Force

The EBS-C section of the EBS Task Force, led by Urs Maeder from the University of Bern, aims at advancing the fundamental understanding of physico-chemical processes in clay or bentonite materials relevant to various aspects of safety assessment. While ultimately a tight integration between EBS-THM and EBS-C is desired, the two EBS sections are currently working on different modeling tasks, and EBS Task Force meetings are jointly held but in separate sessions for THM and C. Also, in contrast to the EBS-THM section, which usually has a tight connection between models and experiments, the "chemical" task force has been mainly working on conceptual model development and modeling benchmark studies of varying complexity. The main goals of the EBS-C section are:

- To develop and test alternate porosity concepts that explain fundamental properties like ion and water transport and swelling pressure in bentonite buffers and other nanoporous materials,
- 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 (integration with EBS-THM). There is presently no THM code available that integrates a full chemical module including an electrostatic treatment of pore water, and likewise there is no general reactive transport code that handles an electrostatic treatment of pore water and is linked to HM processes.

3.4.4.1 Current Modeling Benchmarks

In terms of model comparison, the EBS-C group has been working on benchmark data sets of various complexity based on experiments. While these benchmarks are generally highly idealized and quite simple in terms of geometry, they tackle chemical questions of high complexity. The following provides a brief description of the benchmark data sets used in the EBS-C Task Force.

Benchmark 1: Salt Diffusion in Montmorillonite

This benchmark experiment evaluates diffusion of salts (Na/Ca) through 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 3-74 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 $CaCl_2$ 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 are available through the SKB EBS TF website. The experiments are discussed in Birgersson et al. (2009).

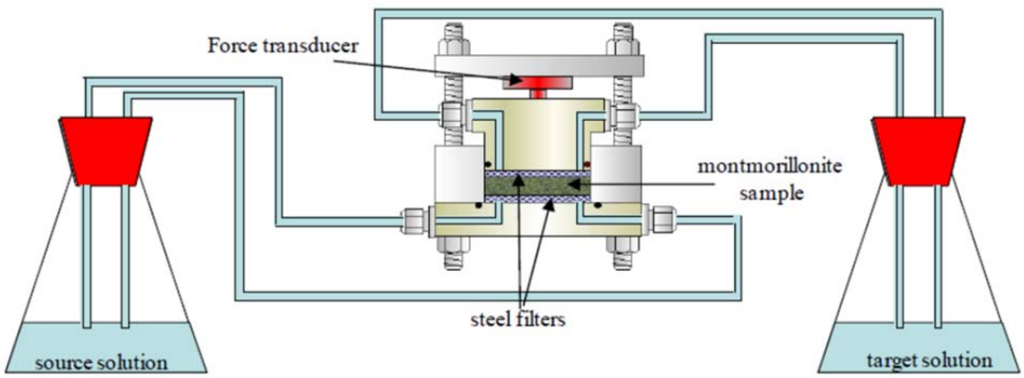


Figure 3-74. Experimental setup for Benchmark 1 involving salt diffusion experiment in montmorillonite (Birgersson, 2011; Birgersson et al., 2009)

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 3-75. 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 conducted by UFD (Cheshire et al., 2014), where degradation of secondary phases could yields marked effects on the altered mineral assemblage and solution chemistry.

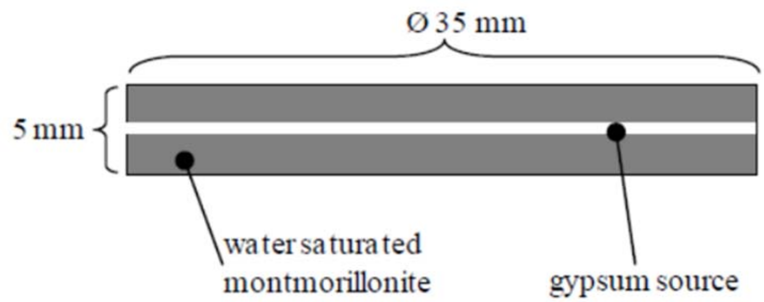


Figure 3-75. Sample configuration for Benchmark 2 experiments (Birgersson, 2011)

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). The purpose of these tests is to evaluation 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 3-76 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).

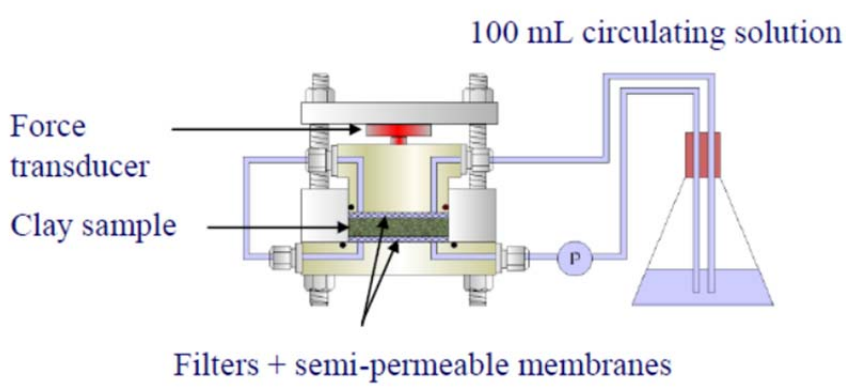


Figure 3-76. Experimental setup for Benchmark 3 to investigate ion exchange and effect on swelling pressure (Birgersson 2011; Birgersson et al., 2009)

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

Benchmark 4 investigates a percolation experiment (Figure 3-77) 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) provided 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.

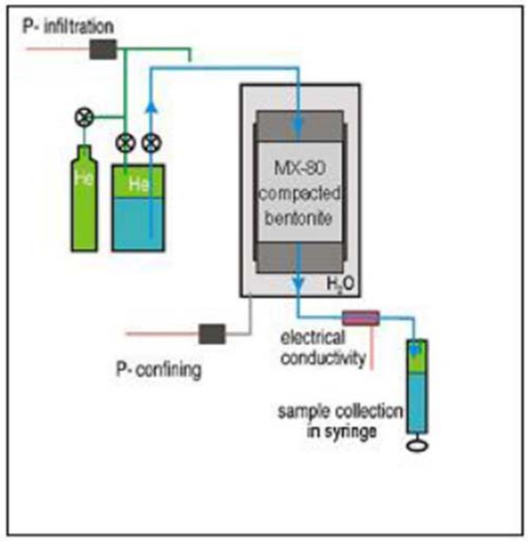


Figure 3-77. Schematic diagram of percolation experiment setup for compacted bentonite (Birgersson, 2011)

<u>Benchmark 5: Diffusion of Selected Anions through Compacted Bentonite</u>

This benchmark describes the diffusion of the anions Cl^-, I^-, and SeO_4^{--} in compacted Czech bentonite (Birgersson, 2011; Hofmanová and Červinka, 2014). Radionuclides of these anionic species ($^{36}Cl^-$, $^{129}I^-$, and $^{79}SeO_4^{--}$) 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 3-78) 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.

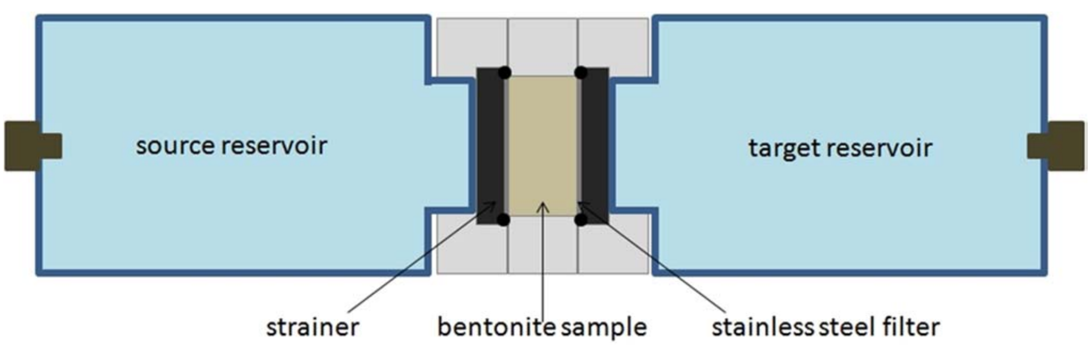


Figure 3-78. Schematic diagram showing diffusion cell used in Benchmark 5 (Birgersson, 2011; Hofmanová and Červinka, 2014)

3.4.4.2 Potential Future EBS-C Tasks and Outlook

The ongoing Benchmarks (1 – 5) provide a platform for collaboration tasks that are aligned with UFD 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 EBS-C Task Force. This work could target sorption dynamics at clay edge sites and diffusion effects using the expertise from the UFD R&D on MD modeling on clay. Another potential activity is the application of density functional theory 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 EBS-C Task Force (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.

In addition, the EBS-C Task Force is presently considering new ideas about future activities and priorities. Below is a list of some of the topics discussed in recent EBS workshops.

- Experiments discriminating among concepts: Recent work has described "up-hill diffusion" of Na across a clay membrane and against a distinct salinity gradient between external reservoirs. Clearly, such behavior cannot be modeled without electrostatic effects that dictate ion equilibrium within the clay. A more difficult issue is to distinguish among the relative merits of the homogeneous mixture model and dual porosity models that treat electrostatic effects in the porosity representing the interlayer volume. There is largely agreement within the Task Force that a proper treatment of ion equilibrium within the interlayer volume (via Donnan approximation to the Poisson-Boltzmann distribution, for example) should be a central element in a conceptual model and its implementation.
- Interlayer chemistry: Accepting that chemistry in swelling clays largely happens within the interlayer space leads to some currently unresolved issues. For example, what type of water is contacting a canister in contact with bentonite? Is it the "free pore water" that exists in dual-porosity models, or is it interlayer water containing much higher concentrations of cations, including protons?
- HM-C coupling: There are relatively few experiments that include a complete description of the pore water chemical aspects and hydromechanical constraints. It is thought that such experiments are needed as test cases for implementing a coupling between chemistry and hydromechanics. Benchmarks 1-4 are also characterized with respect to swelling pressure or total pressure constraints, and could be used in this context. A new initiative by POSIVA (with Uni Bern) aims at providing a comprehensive HMC data set based on new squeezing experiments under drained conditions, as basis for future modeling.

Similar to the EBS-THM task force, there are no final decision yet as to which new task ideas might be carried forward in the EBS-C task force. DOE/UFD will be represented at future task force meetings and will help finalize the future task list of the EBS-C Task Force.

3.4.5 SKB Task Force Summary

Benefits of Participation:

- Access to **several** sets of experimental data from **one** URL in crystalline rock
- Opportunity to perform **modeling and analysis of existing data** in collaboration with other modeling groups (typically less direct interaction with the project teams that run or interpret the experiments)

Status of Participation:

DOE joined both task forces in January 2014. UFD researchers have actively engaged in the interpretation and modeling of a bentonite-rock experiment (Section 6.1.5).

Outlook:

With DOE's membership in the task forces recently formalized, UFD's collaboration portfolio with SKB is still in development. In addition to BRIE, there are other valuable tasks, a selection of which will be conducted in FY16.

Contact Information:

DOE Contact:
Prasad Nair, DOE-NE

UFD Contact:
Jens Birkholzer, LBNL
Hari Viswanathan, LANL (GWFTS Task Force)
Carlos Jove-Colon, SNL, and Liange Zheng, LBNL (EBS Task Force)

SKB Contact:
Anders Sjöland, Executive Secretary, Technical-Scientific Council, SKB, Sweden
Björn Gylling, Secretary of GWFTS Task Force, SKB, Sweden
Antonio Gens, EBS Task Force for THM, from UPC, Spain
Urs Maeder, EBS Task Force for THC, University of Bern, Switzerland

3.5 NEA's Cooperative Initiatives

The previous sections describe initiatives that foster active research with other international disposal programs, provide access to field data, and/or may allow participation in field experiments in URLs (Sections 3.1 to 3.4). Here we briefly touch on NEA's international collaboration initiatives where the focus is less on active collaboration than on the exchange of information and shared approaches.

3.5.1 NEA's Clay Club

In 1991, the Nuclear Energy Agency (NEA) established a "Working Group on the Characterization, the Understanding and the Performance of Argillaceous Rocks as Repository Host Formations," known more commonly as the "Clay Club" (http://www.oecd-nea.org/rwm/clayclub/). Since 2000, the Clay Club has operated under the umbrella of NEA's Integration Group for the Safety Case (IGSC), an international forum on confidence-building in repository technical safety cases and on the underlying methodological and scientific bases for the purpose of decision-making in repository development. The Clay Club promotes the exchange of information and shared approaches and methods to develop and document an understanding of clay media as a host rock for a repository. The Clay Club generally establishes the program of work at its own initiative, based on experience and progress in repository programs of its member countries. The work program and products are presented at each IGSC plenary meeting. The Clay Club may also carry out specific tasks at the request of IGSC dealing with, for instance, the analysis of performance of clays for safety assessment purposes. The Clay Club chooses among a variety of mechanisms for its work program, including, for example: to install task-oriented expert groups; to organize workshops; to hire dedicated consultants and specialists; to collaborate in conferences; or a combination of these. A high priority is placed on making the results of Clay Club projects publicly available, using printed and/or electronic publications. The Clay Club working group is composed of senior technical experts with experience in assembling or reviewing the understanding of argillaceous media as host rocks for deep geologic disposal projects. Members represent waste-management agencies, regulatory authorities, academic institutions, and research and development institutions.

The work program and modus operandi of the Clay Club emphasize the pooling of resources, the sharing and synthesis of understanding and experiences, and the communication of findings to various audiences. Clay Club projects are established most often at the initiative of the members; work may also be undertaken on specific topics at the request of the IGSC. The topics of work reflect issues of common interest, considering the experience, progress and challenges of national program. Decisions on projects are made on a consensus basis, taking into account the importance and urgency of the issue, the breadth of interest (i.e., the number of national program for whom the issue is considered a key issue), and the necessary resources and schedules to accomplish the work proposed. Communication within the group takes place through plenary meetings, which occur on at least an annual basis.

In general, the Clay Club addresses recommendations, trends, and information gaps concerning the characterization, evolution, modeling, and performance of argillaceous media, for example regarding:

- Understanding (and development of associated conceptual models) of argillaceous rocks through site characterization and expert evaluation, including both field and laboratory work on key issues
- Quality (characterization, understanding and conceptualization capability) and limitations of the information that is available
- Performance assessment and supporting models, including model abstraction and simplification as well as the traceability of related data and information
- Links and potential knowledge transfer between the understanding of clay as a host material and its use in engineered barrier systems of geologic repositories

- Relevant progress in R&D on clay materials in other fields or industries, such as petroleum exploration and CO_2 sequestration

Examples of topics that have been (or are being) addressed are:

- Catalogue of characteristics of the various argillaceous media;
- Relevant FEPs
- Use of natural tracers to support long-term dominance of diffusion;
- Role and influence of faults and fractures at repository depths
- The quality and limitations of the information that is available
- Potential for self- sealing of fractures in clay rocks
- Imaging and observations of clays at the microscopic level (current)
- Anomalous heads in clay media (current)
- Micro-mechanical models (current)

Membership in the Clay Club requires no formal agreement, but rather a simple expression of interest, acceptance by current Clay Club members, and a voluntary annual financial contribution. Each member organization sends a representative to the annual meetings and provides a report on ongoing activities. Clay Club members are expected to: promote Clay Club activities in their own organization; provide relevant data and bibliographic material to support Clay Club initiatives; and, as appropriate and on an ad hoc basis, make human or financial resources available to the Clay Club initiatives. In contrast to other international initiatives (such as the Mont Terri Project, DECOVALEX, or SKB's Task Forces), the Clay Club is not about active R&D collaboration, but rather about having a regular forum for in-depth discussion and information exchange. Current members are institutions from Belgium, Canada, France, Germany, Hungary, Japan, Netherlands, Spain, Switzerland, and United Kingdom. DOE has been contemplating membership in the past, but so far has not ultimately decided on participation.

3.5.2 NEA's Salt Club

The Salt Club brings together nations currently considering rock salt as a candidate medium for deep geologic disposal of HLW and long-lived radioactive waste (http://www.oecd-nea.org/rwm/saltclub/). The club's mission is to develop and exchange scientific information on rock salt as a host rock formation for deep geologic repositories. By promoting information and knowledge exchange, the Salt Club also intends to stimulate interest in other nations with appreciable rock salt deposits to consider rock salt as a viable repository medium. In addition to the technical aspects, the working group also aims at transferring obtained knowledge to programs at different phases of development, fostering education and training of future subject-matter experts in the field of rock salt, and cooperating with other NEA working groups (e.g., the Forum on Stakeholder Confidence, FSC) to engender public acceptance and building stakeholder confidence. The Salt Club working group is composed of senior technical experts with experience in assembling or reviewing the understanding of salt formations as host rock for deep geologic disposal projects. Members represent waste management agencies, regulatory authorities, academic institutions, and research and development institutions. Salt Club members have a level of seniority in their organizations such that they are able to mobilize resources to contribute to Salt Club initiatives. DOE is a current member of the Salt Club; other members are Sandia National Laboratories (SNL), Los Alamos National Laboratory (LANL), and institutions from Germany, the Netherlands, and Poland.

The club started in 2011 as a NEA working group, comprised of scientists and experts in developing disposal in geologic rock salt formations. The official kick-off meeting for the Salt Club took place on April 20, 2012, at the OECD NEA headquarters in Paris to discuss initial work activities, schedules and other project details. Recently, the 4th Nuclear Energy Agency (NEA) Salt Club Meeting was held February 25, 2015 in Paris, France. The Salt Club has the following areas of interest:

- Geomechanical issues (coupled processes, excavation damaged zone (EDZ) behavior, rock mechanic issues, backfilling, sealing and plugging of rooms, drifts, shafts)
- Brine and gas migration
- Actinide and brine chemistry
- Microbial activities in rock salt
- Geochemical issues (radionuclide chemistry, modeling, natural analogs)
- Technical/technological and engineering issues (construction, operation, closure)
- Performance of geotechnical barriers
- Contributions to the Safety Case (e.g. FEP catalog, scenarios, performance assessment issues, uncertainties, use of natural analogs)

Similar to the Clay Club, the Salt Club is not about active R&D collaboration, but rather about providing a regular forum for in-depth discussion and information exchange.

3.5.3 NEA's Thermochemical Database Project

The purpose of the international Thermochemical Database Project (TDB) is to make available a comprehensive, internally consistent, quality-assured and internationally recognized chemical thermodynamic database of selected chemical elements, in order to meet the specialized modeling requirements for safety assessments of radioactive waste disposal systems. The unique feature of the TDB project is that the data are evaluated and selected by teams of leading experts drawn from universities and research institutes around the world, through a critical review of the existing primary experimental sources. Detailed TDB reports document the process leading to the selected values. Participating countries are as follows: Belgium, Canada, Czech Republic, Finland, France, Germany, Japan, Spain, Sweden, Switzerland, United Kingdom, and the United States. A history of NEA TDB activities was recently published and summarizes the accomplishment of the project since its inception in 1984 (Ragoussi and Brassinnes, 2015).

The project has operated in five phases over almost two decades. During the first part of the project, a high priority was assigned to the critical evaluation of the data of inorganic compounds and complexes of the actinides uranium, americium, neptunium, and plutonium, as well as the inorganic compounds and complexes of technetium. The second phase provided for further needs of the radioactive-waste-management programs by updating the existing database and applying the TDB methodology to new elements present in radioactive waste (as fission or activation products): nickel, selenium and zirconium, and also simple organic complexes. The third phase started in 2003, with three new reviews on thorium, tin, and iron (part 1), and with the constitution of an expert team for the preparation of guidelines for the evaluation of thermodynamic data for solid solutions. The fourth phase (2008-2013), included three reviews concerning molybdenum, iron (part 2) and ancillary data, and the initiation of two state-of-the-art reports on cement minerals and high-ionic-strength solutions. The program for the current fifth phase (2014-2018) of the Thermochemical Database (TDB) Project comprises the following activities:

- Completion of the reviews from the fourth phase
- Preparation of an update of the phase II actinide volumes, including technetium
- Preparation of a state-of-the-art report on the thermodynamic properties of cement minerals
- Preparation of a state-of-the-art report on thermodynamic considerations for actinides in high-ionic-strength solutions

DOE has been participating in the TDB Project for a while, and is currently represented by scientists from LLNL.

4. BILATERAL COLLABORATION OPPORTUNITIES

Access to data from international field experiments and participation of UFD researchers in collaborative field studies can also be facilitated via direct informal or semi-formal agreements between national laboratories and international partners. Several UFD scientists have close relationships with their international counterparts, resulting from workshops and symposia meetings, or from collaboration outside of UFD's scope. International disposal programs benefited from collaboration with UFD scientists and are generally quite open to including them in their ongoing research teams. This may require preparation of MoUs or other types of bilateral agreements. The U.S. DOE has several such bilateral agreements in place, among those the Joint Fuel Cycle Studies (JFCS) agreement with the Republic of Korea, with the German Federal Ministry of Education and Research (BMWi), with Japan under the JNEAP (Joint U.S.–Japan Nuclear Energy Action Plan) agreement, and with France as a result of a recent MoU with ANDRA. The subsections below give a short description of selected bilateral collaboration opportunities providing access to valuable data and major field experiments. The first two opportunities with the Republic of Korea and Germany have already resulted in close collaborative research work between UFD scientists and their international counterparts; the others describe opportunities for future collaboration. This list will be amended and updated as new opportunities arise.

4.1 Experiments at KURT URL, Republic of Korea

KURT is a generic underground research laboratory hosted by a shallow tunnel in a granite host rock, located in a mountainous area near Daejeon, Republic of Korea. KURT stands for KAERI Underground Research Tunnel, with KAERI being the Korea Atomic Energy Research Institute. Using KURT, KAERI intends to obtain information on the geologic environment and the behavior and performance of engineered barriers under repository conditions. KURT has a total length of 255 m with a 180 m long access tunnel and two research modules with a total length of 75 m. The maximum depth of the tunnel is 90 m from the peak of a mountain. The horseshoe shape tunnel is 6 m wide and 6 m high (Figure 4-1). The tunnel construction at KURT started in March 2005 and was completed in November 2006. An expansion of the tunnel has recently been completed as shown in Figure 4-2, which allows for additional several hundred meters of tunnel length for further site characterization and *in situ* testing. The host rock is granite, which is one of the potential host rock types for an HLW disposal repository in Korea. The utilization of radioactive material in KURT is not allowed.

Compared to other URLs, including those discussed in Section 3, KURT is a relatively new facility. The first 5-year research phase started in 2006 after successful completion of the facility. Past or current research works has included (1) geologic characterization and long-term monitoring, (2) development and testing of site investigation techniques, (3) solute and colloid migration experiments, (4) EDZ characterization, (5) borehole heater tests, and (6) investigation of correlation between streaming potential and groundwater flow (Figure 4-3). A second 5-year research phase, which started in 2012, comprises additional site characterization work related to the tunnel expansion and *in situ* long-term performance tests on a 1/3 scale engineered barrier system at KURT. The focus of the site characterization work is a major water-conducting feature (MWCF), which was initially identified from surface boreholes and which will soon be accessed from the new expansion tunnels. The hydrogeological, geochemical, and transport properties of the MWCF will be characterized, before, during, and after excavation.

The KURT site offers one unique feature with regards to *in situ* borehole characterization and deep borehole disposal R&D. The site hosts an existing deep (1 km) borehole drilled into granitic bedrock, which provides a unique opportunity for developing and testing techniques for *in situ* borehole characterization in fractured crystalline rocks. The DB-2 borehole was drilled from the surface to a depth just outside of the KURT facility (Figure 4-4) to better understand the deep geologic, hydrogeological, and chemical characteristics around the KURT site, and to specifically explore the MWCF. The deep borehole could offer possibilities of collaboration regarding deep borehole disposal concepts. The Republic of Korea and KAERI are interested in further exploration of deep borehole disposal concepts.

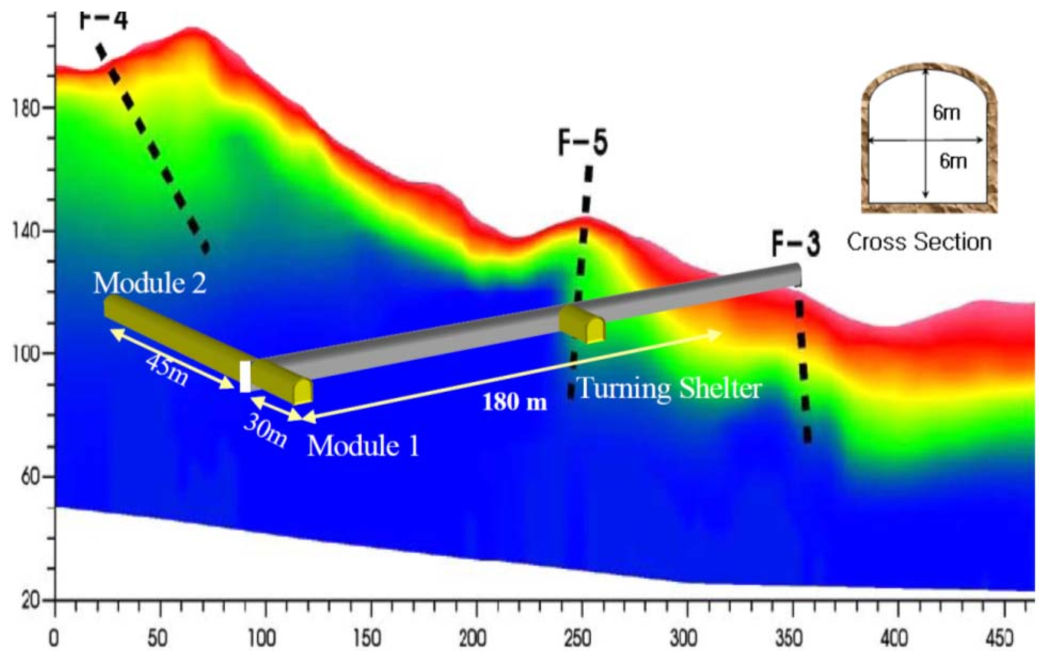


Figure 4-1. Current layout of the KURT URL in Daejeon, Korea (from KAERI, 2011)

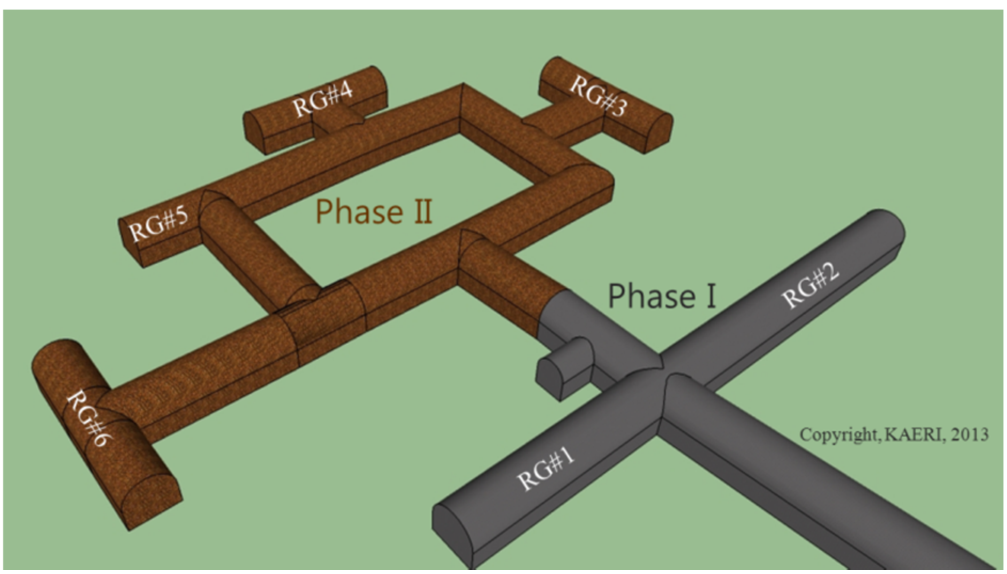


Figure 4-2. Preliminary layout for tunnel extension of KURT (from Wang et al., 2014)

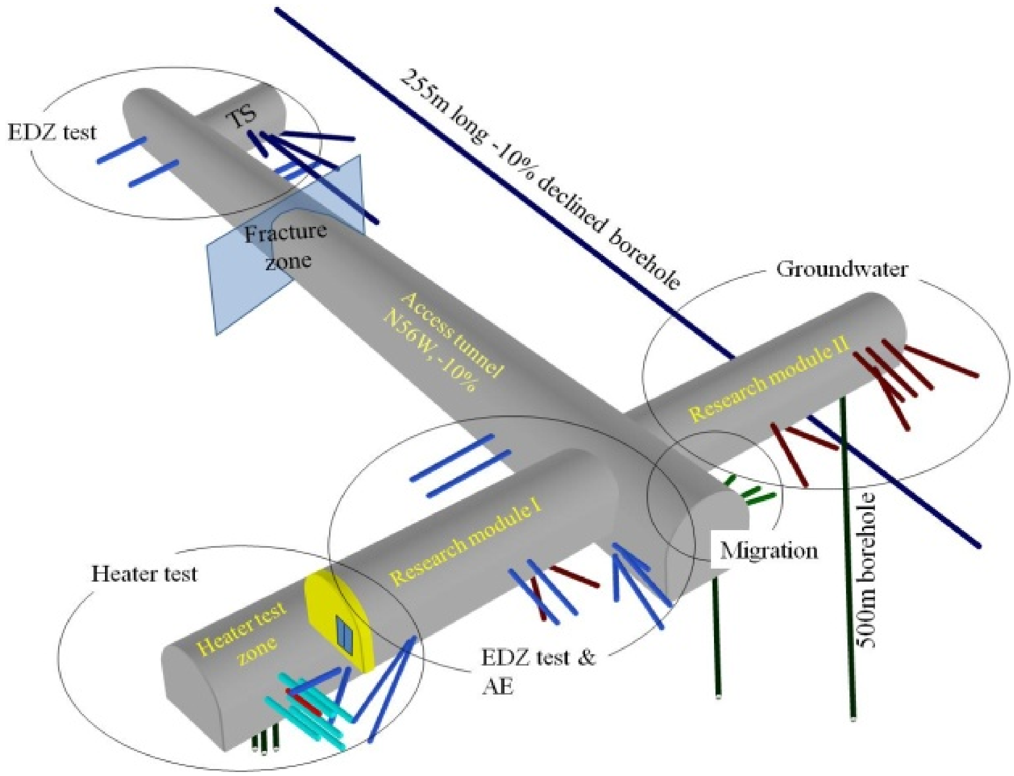


Figure 4-3. Location of *in situ* tests and experiments with related boreholes at KURT (from Wang et al., 2014)

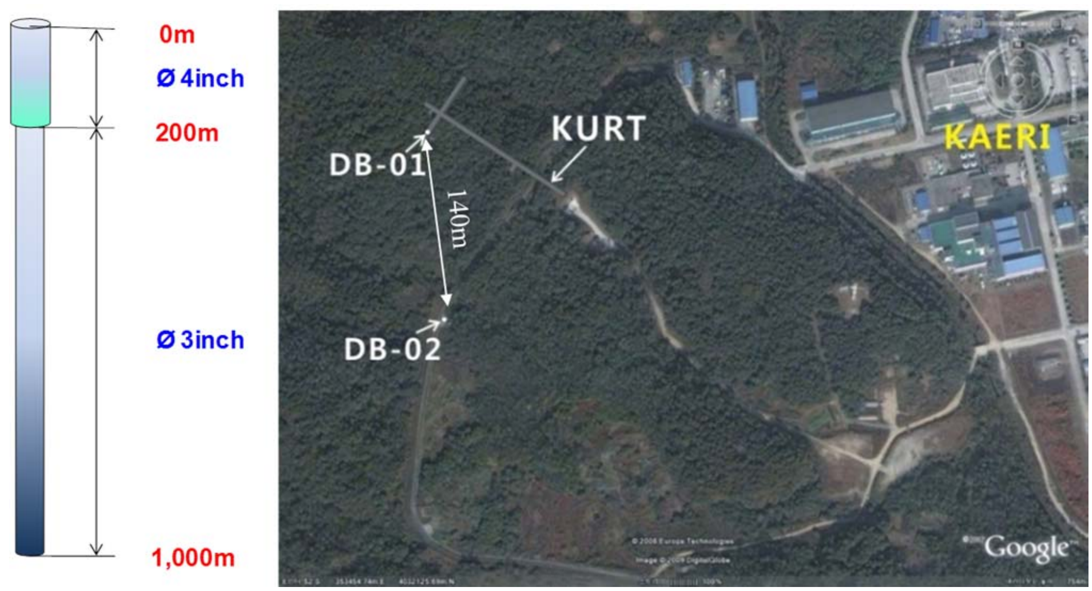


Figure 4-4. Specification of DB-2 borehole and its location near KURT site (from Wang et al., 2014)

In general, KAERI is open to international collaboration and is looking for new ideas and experimental designs for future tests. A few years ago, a formal commitment to collaboration on the management of nuclear fuel was established between the United States and the Republic of Korea (ROK). The agreement, called the Joint Fuel Cycle Studies (JFCS), between the U.S. Department of Energy, the ROK Ministry of Education, Science & Technology, and the ROK Ministry of Knowledge Economy, focuses mainly on three areas of fuel-cycle technologies (electrochemical recycling, safeguards, and fuel cycle alternatives), but has also some research elements related to geologic disposal. Researchers at SNL and KAERI have developed a multi-year plan for joint field testing and modeling to support the study of high-level nuclear waste disposal in crystalline geologic media, which includes sharing of KURT site characterization data. There are two specific collaborative tasks, as follows: (1) streaming potential (SP) testing regarding correlation with groundwater flow, and (2) technique development for *in situ* borehole characterization. For Task 1, KAERI and SNL have completed the experimental design and conducted a first set of laboratory tests. *In situ* testing is planned at KURT once the extension is completed. For Task 2, KAERI and SNL have finalized a new contract for collaborative work on the development of in-situ hydrological and geochemical measurements in boreholes. This task is a joint effort between the UFD deep borehole disposal work package and the crystalline disposal R&D work package. More detail on these collaborative tasks is given in Section 6.3.1.

4.2 Salt Research Collaboration with German Researchers

DOE/UFD scientists and their German colleagues in academia and other research laboratories collaborate closely on various R&D issues related to disposal of radionuclide waste in salt. A MoU was signed a few years ago between DOE and the German Federal Ministry of Economics and Technology (BMWi) to cooperate in the field of geologic disposal of radioactive wastes (MoU date: November 2011). Four U.S. –German Salt workshops have been held so far to advance collaboration, starting with a preparatory workshop on May 25–27, 2010, in Jackson Mississippi, followed by Peine, Germany, (November 9–10, 2011), Albuquerque, New Mexico (October 8–11, 2012), Berlin, Germany (September 16–17, 2013) (Hansen et al., 2013), and Santa Fe, New Mexico (September 8-10, 2014) (Hansen et al., 2015). The overriding premise for U.S./German collaborations is to advance the scientific basis for salt repositories. Today, scientists from both countries have started cooperative work in several areas, including coupled-salt-mechanics modeling (Section 6.1.6), safety case aspects, plugging and sealing of a salt repository, and repository design (see Section 7.1).

Germany has a long history of salt R&D. The country started in 1979 to conduct exploration work at the Gorleben salt dome to evaluate its suitability for waste disposal (Figure 4-5). However, a moratorium on further exploration at the Gorleben site was imposed in 2000, mainly due to political reasons. While the moratorium has now been lifted, R&D activities at Gorleben have not yet resumed, and it is questionable whether and when further underground testing at this URL might be conducted. Another mine, the Asse II mine, was also used as a research facility in the past, between 1965 and 1995, where some major experiments such as the long-term TSDE (*Thermal Simulation for Drift Emplacement*) experiment were carried out. As shown in Figure 4-6, the TSDE experiment comprised of two parallel drifts, each of which housing three electrical heaters to simulate emplacement of heat-producing waste. A significant amount of data was collected over several years in 20 monitoring cross sections: temperature, stress changes, displacement, convergence, and porosity of crushed salt, among others. Data from the TDSE experiment are currently used by UFD scientists to validate the large-scale applicability of coupled THM models (Rutqvist et al., 2015). Note that between 1967 and 1978, low-level and intermediate-level radioactive wastes were placed in storage in other parts of the Asse II mine. Research was eventually stopped; between 1995 and 2004, all underground tunnels and cavities were filled with salt. Today, the Asse II mine is the subject of major controversy because of security concerns regarding water inflow and salt stability.

Figure 4-5. View of one of the underground tunnels at Gorleben site at the 840 m level (from BMWi, 2008)

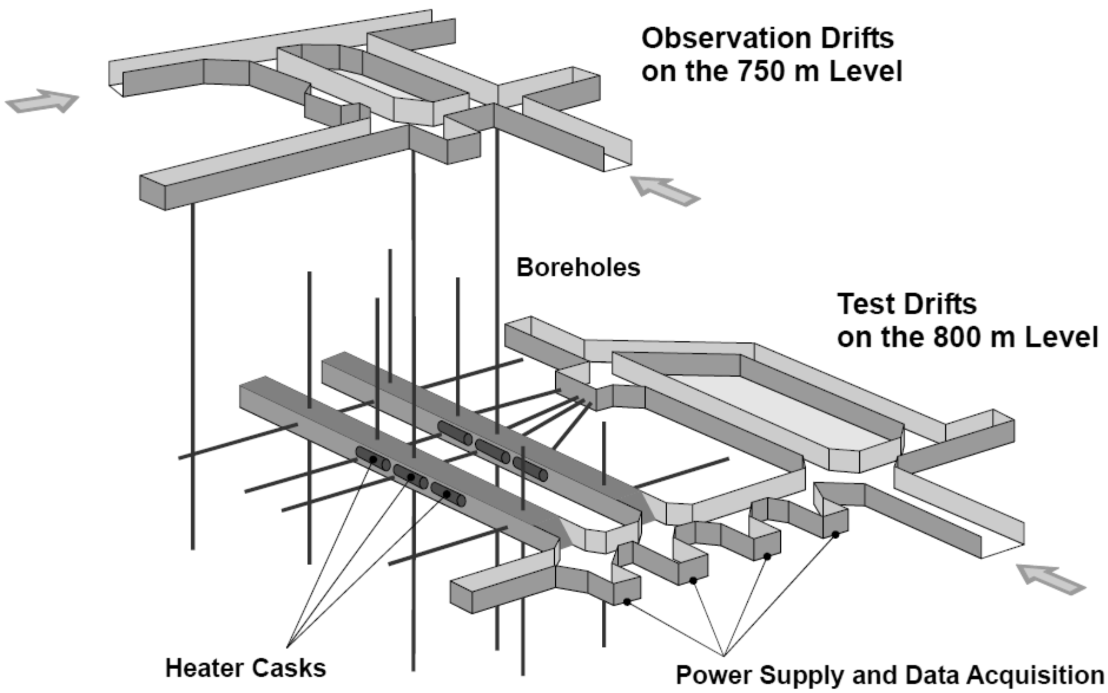


Figure 4-6. Schematic view of the two drift tests used in the TSDE experiment (800 m level of the Asse salt mine) (from Ruqvist et al., 2015)

4.3 Collaboration Opportunities at ANDRA's LSMHM URL, France

The major underground disposal research facility in France is ANDRA's LSMHM URL sited near Bure in the Meuse and Haute-Marne districts in the east of France, co-located with the proposed French disposal site Cigeo. R&D at Bure aims at studying the feasibility of reversible geologic disposal of high-level and long-lived intermediate-level radioactive waste in the Callovo-Oxfordian clay formation. This facility was licensed in August 1999, and its construction (access shafts, basic drift network with underground ventilation) was finalized in 2006. As shown in Figure 4-7, the URL consists of two shafts sunk down to a depth of about 500 m. A network of about 900 m of tunnels and drifts is used for various scientific experiments, engineering technological demonstrations, and the testing of industrial solutions for construction and operation (Figure 4-8). A recent MoU between ANDRA and DOE can be a starting point for collaborative work in clay/shale disposal at the Bure URL, though currently there are no ongoing joint R&D projects between U.S. and French scientists related to the Bure URL. Note that ANDRA has tentatively proposed to utilize its Alveole Heater Test as one possible test case for the new DECOVALEX-2019 phase starting in 2016 (see Section 3.1.3.5).

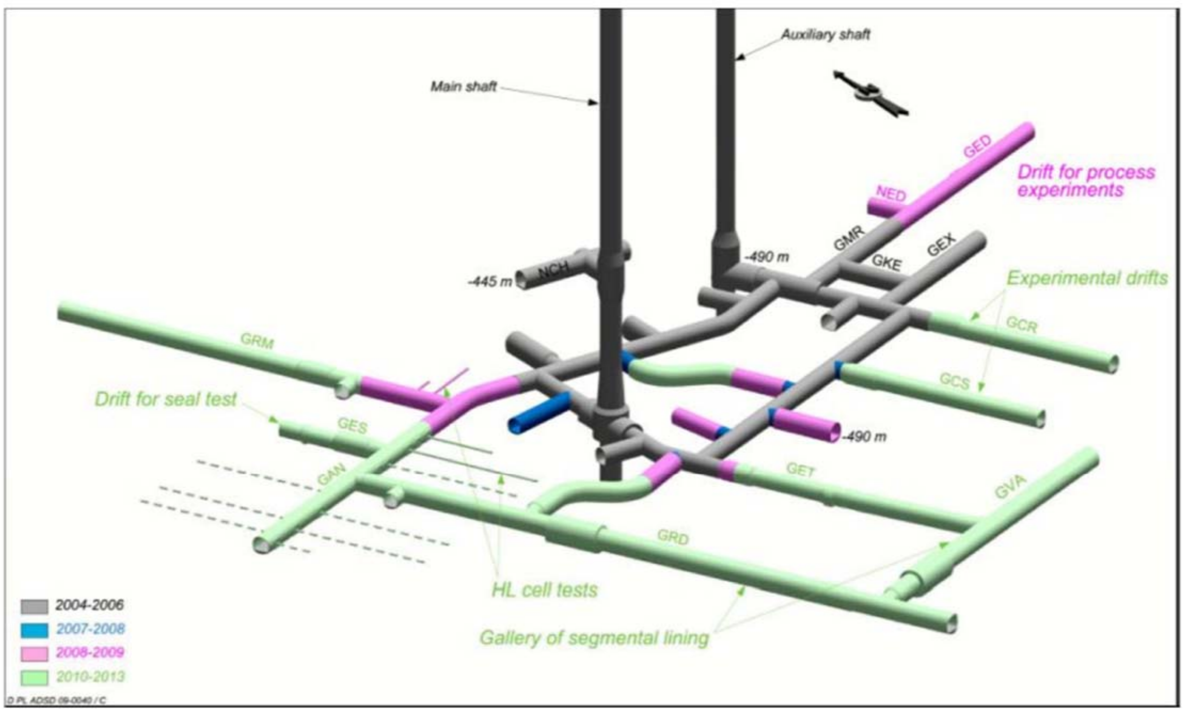


Figure 4-7. Layout of the LSMHM URL at Bure, France (from Lebon, 2011)

Figure 4-8. LSMHM URL at Bure, France (from http://www.andra.fr/download/andra-international-en/document/355VA-B.pdf)

4.4 Collaboration Opportunities with JAEA's URLs in Japan

Opportunities for active collaborative R&D with Japan exist not only at the Horonobe URL in sedimentary rock (see Section 3.1.2.3), but also at this nation's second URL at the Mizunami Underground Research Laboratory, which resides in crystalline rock (Figure 4-9). Japan and the United States entertain close collaboration on issues related to nuclear energy under the JNEAP (Joint U.S.–Japan Nuclear Energy Action Plan) agreement. JNEAP has a Waste Management Working Group that meets in regular intervals to discuss joint R&D on, among other topics, waste disposal issues. Japanese research institutions are also a frequent partner in many of the cooperative initiatives that DOE has joined in recent years (see Section 3, Table 3.1), and both nations collaborate on the DECOVALEX task featuring JAEA's Horonobe EBS experiment. There are currently no joint activities related to experimental work at the Mizunami URL. However, JAEA has tentatively proposed to utilize its GREET experiment at Mizunami URL as one possible test case for the new DECOVALEX-2019 phase starting in 2016 (see Section 3.1.3.3).

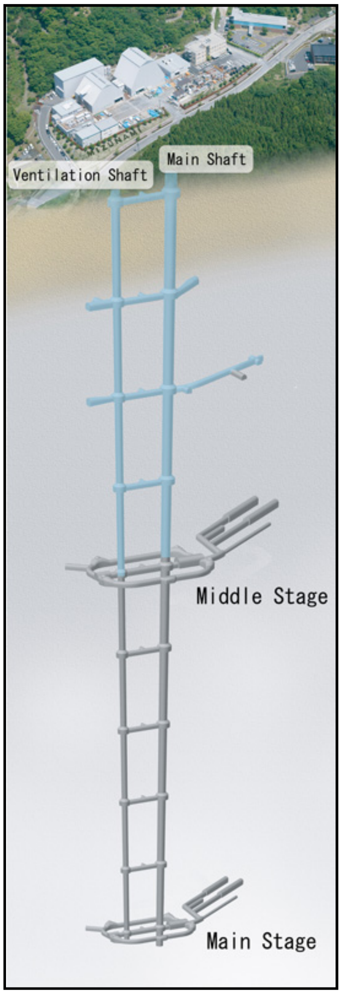


Figure 4-9. Layout of the Mizunami Underground Research Laboratory in Japan, and photo of tunnel shaft construction (from http://www.jaea.go.jp/04/tono/miu_e/)

4.5 Collaboration Opportunities at HADES URL, Belgium

Belgium is another country with a strong R&D program in geologic disposal and a long history of experimental work in an underground research laboratory. The HADES (High Activity Disposal Experimental Site) URL is located in a secured area belonging to one of Belgium's nuclear power plants, which also hosts other nuclear research facilities. HADES is essentially a several-hundred-meter-long tunnel in the soft Boom Clay rock formation, accessible by two shafts located at each end (Figure 4-10). The tunnels were drilled in stages, starting with a first section in 1982, followed by additions in 1987 and 2001. Each of these sections was secured with different types of ground support, reflecting increased knowledge about the structural behavior of the host rock. Most interesting to DOE's program is probably the PRACLAY heater experiment, and to a lesser degree long-term clay diffusion experiments, both of which are discussed in more detail below. The Belgium organizations involved in conducting and interpreting these experiments have long-standing relationships with DOE/UFD scientists; they are open to participation with UFD research groups and have already invited researchers to provide THM modeling expertise to the PRACLAY project team. However, there are currently no joint activities related to the HADES URL.

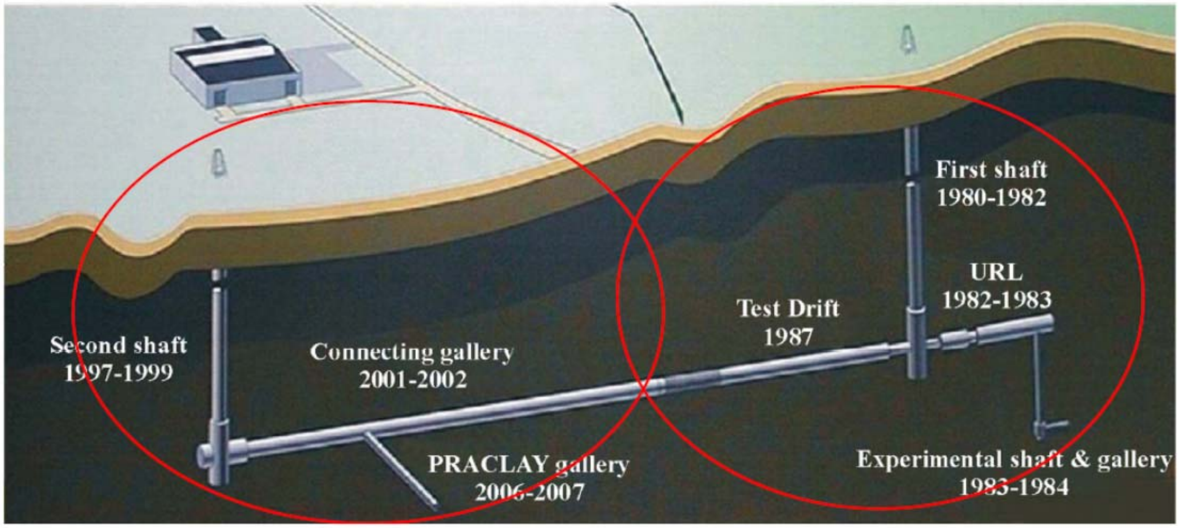


Figure 4-10. Layout of the HADES URL in Mol, Belgium (from Li, 2011)

4.5.1 PRACLAY Test

The PRACLAY Heater Test is a full-scale validation and confirmation experiment conducted at the HADES URL, excavated at 223 m depth in Boom Clay, a tertiary clay formation in Mol, Belgium. The heater test, which started its heating phase in January 2015, involves a 30 m gallery section heated for 10 years with many monitoring sensors (Figures 4-11, 4-12, and 4-13), for the purpose of investigating the thermo-hydro-mechanical (THM) behavior of near-field plastic clay under the most "mechanically critical" conditions that may occur around a repository (Van Marcke and Bastiaens, 2010). For plastic clay under the influence of temperature change, these are undrained conditions, which then generate a higher pore-pressure increase and a higher possibility of near-field damage. For this objective, a hydraulic seal has been installed at the intersection between the planned heated and unheated sections of the gallery. This installation makes up the Seal Test, which was initiated in 2010, and allows for testing the functionality of the hydraulic seal under heated repository conditions.

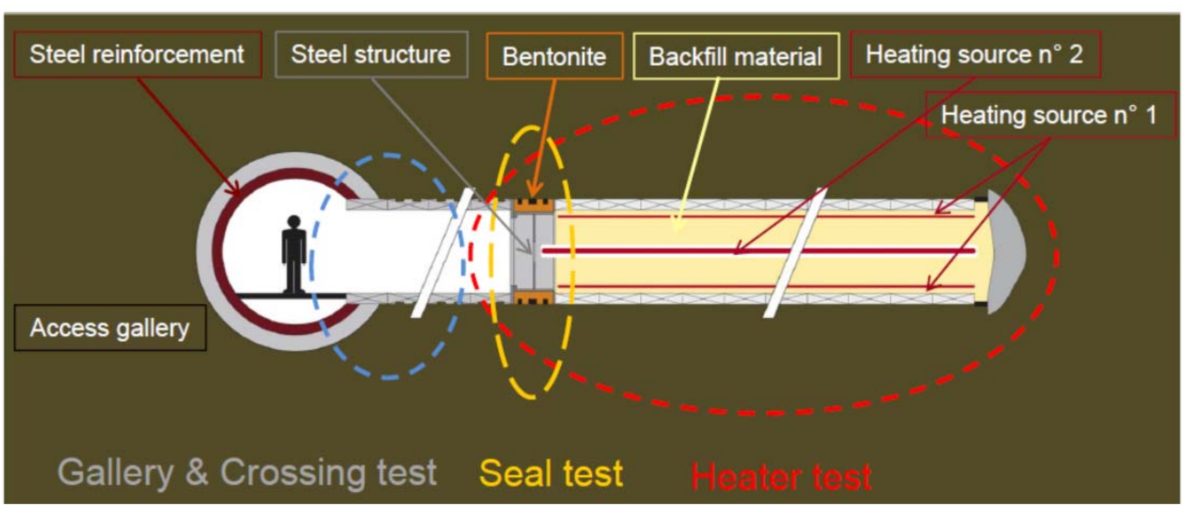


Figure 4-11. Layout of the PRACLAY *in situ* experiment at HADES URL (from Li, 2011)

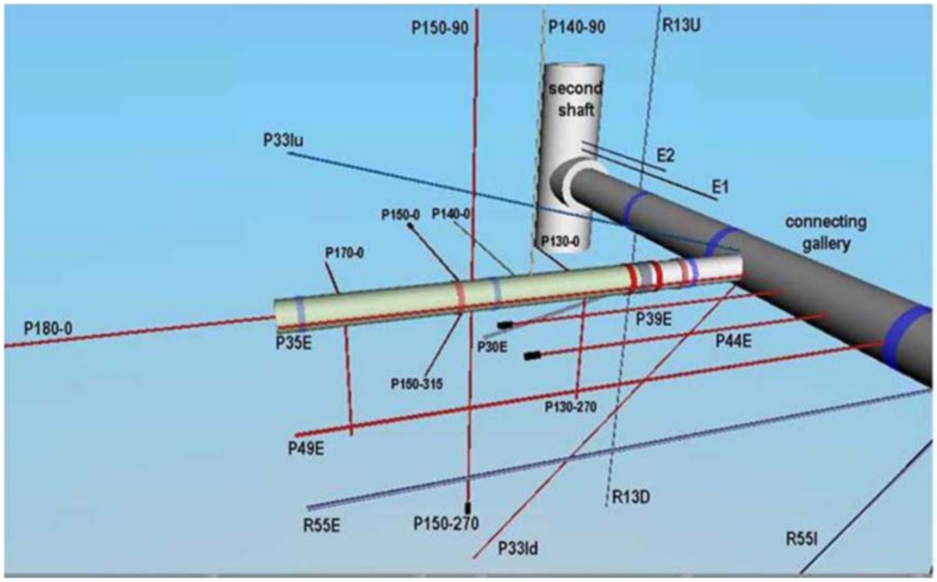


Figure 4-12. PRACLAY *in situ* experiment at HADES URL: Configuration of boreholes for pressure, stress, displacement, and water chemistry measurements (from Li, 2011)

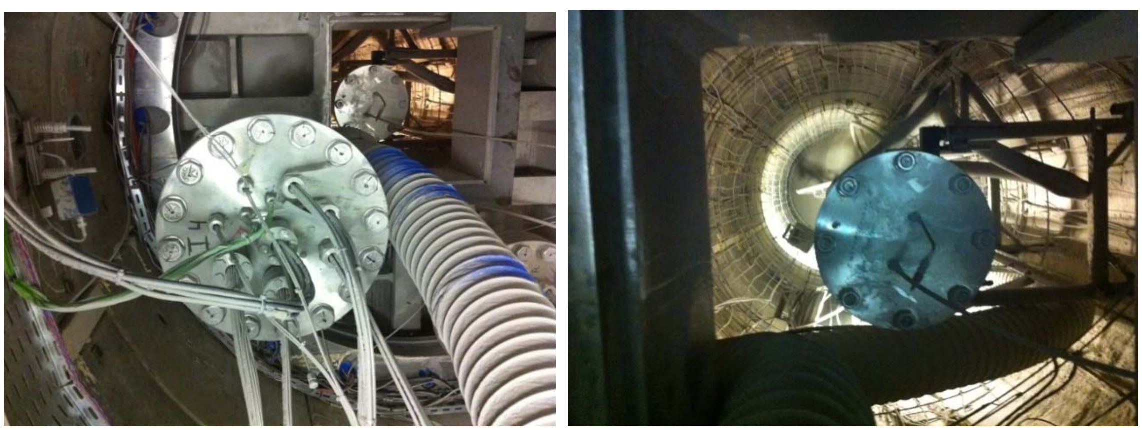


Figure 4-13. PRACLAY *in situ* experiment at HADES URL: Photo on left shows hydraulic seal from the outside, with an access hole to the right, which soon will be closed. Photo on right was taken from access hole into the heater gallery section, which is currently being backfilled.

4.5.2 Radionuclide Migration Experiments

The Belgium waste management program has been conducting a suite of long-term radionuclide migration *in situ* experiments in dense clays at their HADES URL near Mol. Two of these experiments, named CP1 (Figure 4-14) and Tribicarb-3D, have been ongoing for 23 and 16 years, respectively, and offer valuable data on the slow diffusion-controlled migration of radionuclides in clay rock. Because of their duration, they offer unique test cases for model and process validation. Recently, two other ongoing large-scale migration experiments were initiated at HADES. The TRANCOM test involves colloid transport with C-14 labeled humic substances. The RESEAL shaft seal experiment investigates transport of iodine-125 through the disturbed zone and the interface between Boom Clay and bentonite.

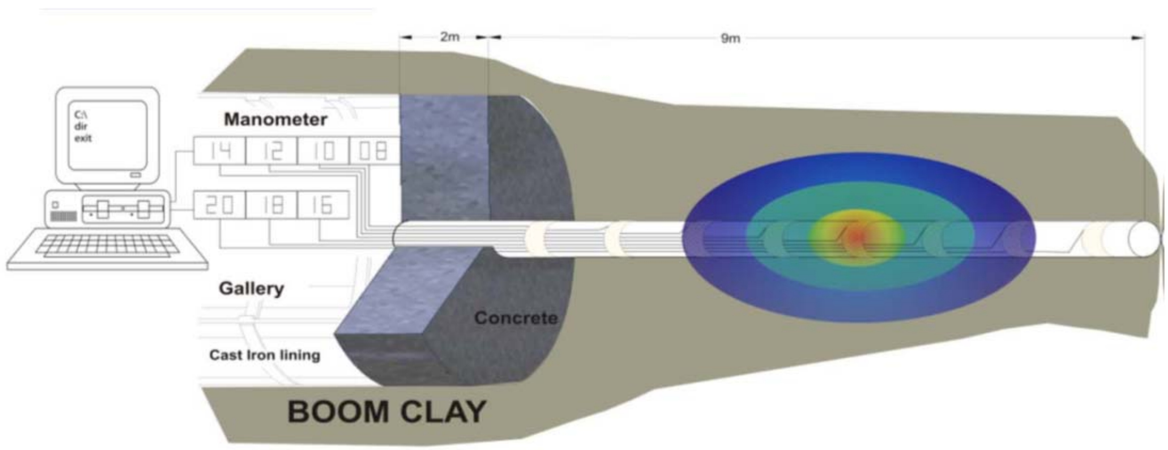


Figure 4-14. Schematic of CP1 Diffusion Experiment at HADES URL (from Maes et al., 2011)

4.6 Collaboration Opportunities at Onkalo URL, Finland

The Onkalo URL in Finland is located at a site chosen to potentially co-host a repository. Thus, it is not only an underground research laboratory, but also an underground characterization facility. It is constructed in crystalline bedrock to the anticipated repository depth of 430–440 m. Construction began in 2004 and is ongoing, but actual underground tests were already started in 2007. Figure 4-15 shows the layout of the URL, with an access tunnel and three shafts. The access tunnel takes the form of a spiral on an approximately 1 in 10 incline downward, and reaches the technical facilities level at about 437 m. The three shafts consist of one personnel shaft and two ventilation shafts. Details may be found in Posiva (2011) and Aalto et al. (2009). There are currently no joint activities between DOE and the Finnish waste management program related to the Onkalo URL. However, the REPRO diffusion experiment at Onkalo is being considered as a new Task 9 in the SKB GWFTS Task Force (see Section 3.4.2.2).

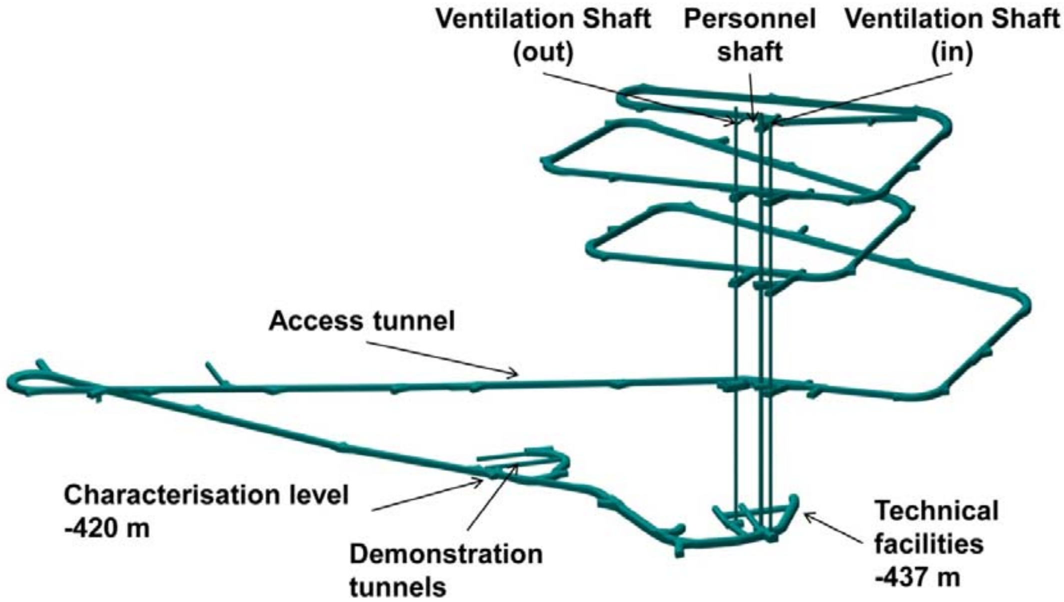


Figure 4-15. Layout of the Onkalo URL in Finland (from Äikäs, 2011)

5. SELECTION OF INTERNATIONAL COLLABORATION TASKS

As discussed in Sections 3, DOE joined several multinational and multipartner initiatives that promote active international collaboration with specific focus on URL field experiments and related data: the DECOVALEX project, the Mont Terri Project, the Colloid Formation and Migration Project (until July 2015), the FEBEX-DP Project, and the SKB Task Forces. UFD researchers are in a position that allows participation in planning, conducting, and interpreting the many past and ongoing field experiments associated with these initiatives, and they do so in close collaborative partnership with international scientists. DOE also reached out to—and explored options of collaboration with—individual international disposal programs, such as the Republic of Korea's KAERI, Germany's BMWi, France's ANDRA, Japan's JAEA, Belgium's SCK/CEN, and Finland's POSIVA (Section 4).

With many collaboration opportunities available to UFD, the campaign in FY12 started a planning exercise to identify the most relevant and promising ones, and to select and develop a set of activities that align with current goals, priorities, and funding plans of the UFD. In a general sense, the benefits of international collaboration are obvious: UFD can gain substantial value from the knowledge, data, and modeling capabilities that international partners have developed over decades of research. However, the benefit of international collaboration needs to be evaluated in the context of the open R&D issues that can be addressed through collaborative scientific activities. Open R&D issues with respect to NBS behavior are summarized in previous progress reports (e.g., *Natural System Evaluation and Tool Development – FY10 Progress Report, August 2010* [Wang, 2010]); specific R&D issues related to clay/shale host rock are discussed, for example, in Tsang et al. (2011). EBS-related R&D items have also been considered in previous progress reports (e.g., Jove-Colon et al., 2010). All R&D gaps identified in these reports have been evaluated in consideration of their importance to the safety case in a roadmap exercise (*Used Fuel Disposition Campaign Disposal Research and Development Roadmap, FCRD-USED-2011-000065 Rev 0, March 2011; Tables 7 and 8;* [Nutt, 2011]).

A summary table was developed in 2012 to provide a basis for planning and selection of international activities. Table 5-1 below is an updated version of this summary table (status September 2014); it lists the most relevant ongoing or planned field experiments conducted in international URLs, provides information on how UFD participation can be achieved, which research areas would be the main benefactor (generally either the Engineered barrier System, EBS, or Natural Barrier System, EBS), the key FEPs addressed (including a link to roadmap and FEPs importance ranking; using the *Used Fuel Disposition Campaign Disposal Research and Development Roadmap, FCRD-USED-2011-000065 Rev 0, March 2011* [Nutt, 2011]), and finally information on the experimental schedules.

Three workshops were held in FY11 and FY12 to inform the DOE leadership and UFD scientists about existing or future international opportunities, and align UFD work-package activities with international initiatives. The first workshop was a session held in conjunction with the UFD Working Group Meeting in Las Vegas, July 12–14, 2011, at this point mostly for informative purposes. The second workshop, held in Las Vegas on April 11, 2012, was a full-day meeting to review the current and planned work scope within UFD work packages for possible leveraging with the international programs, and to develop an initial set of R&D activities that align with goals, priorities, and funded plans of the UFD program. A third workshop was a session held in conjunction with the UFD Working Group Meeting in Las Vegas, May 15–17, 2012, to inform UFD researchers about the outcome of the full-day planning workshop.

Today, three years after its initiation, the international disposal program within UFD has established a balanced portfolio of selected collaborative R&D activities in disposal science, addressing relevant R&D challenges and open research questions as follows:

- Near-Field Perturbation: How important is the near-field damage to a host rock (such as clay and salt) due to initial mechanical and thermal perturbation, and how effective is healing and sealing of the damage zone in the long term? How reliable are existing constitutive models describing the deformation of elastoplastic and plastic geomaterials as affected by temperature and water content changes?
- Engineered Barrier Integrity: What is the long-term stability and retention capability of backfills and seals? In a clay host rock, can bentonite mixtures be developed that allow for gas pressure release while maintaining sealing properties for water? In fractured granite, can bentonite be eroded when in contact with water from flowing fractures? How relevant are interactions between engineered and natural barrier materials, such as metal-bentonite-cement interactions?
- Radionuclide Transport: Can the radionuclide transport in fractured granites be predicted with confidence? What is the potential for enhanced transport with colloids? How can the diffusive transport processes in nanopore materials such as compacted clays and bentonites best be described? What is the effect of high temperature on the swelling and sorption characteristics of clays?
- Demonstration of Integrated System Behavior: Can the behavior of an entire repository system, including all engineered and natural barriers and their interaction, be demonstrated, and is the planned construction/emplacement method feasible?

Table 5-2 summarizes the FY15 portfolio of recent, ongoing or planned UFD activities related to relevant experiments in international URLs. As described in the following sections, this collaborative research portfolio has led to significant advances over the past years. The joint R&D with international researchers and the access to relevant data/experiments from a variety of URLs and host rocks have helped UFD researchers to significantly improve their understanding of the current technical basis for disposal in a range of potential host-rock environments and has contributed to testing and validating predictive computational models for evaluation of disposal-system performance in a variety of generic disposal-system concepts.

Over the years, as research priorities change, and as new opportunities for collaboration develop, UFD's international research portfolio has evolved and will continue to evolve. In FY15, UFD made a targeted effort to re-evaluate its international collaboration activities, in a process similar to the initial planning phase in 2012. Two planning sessions were held in conjunction with the UFD Working Group Meeting in Las Vegas, June 9–11, 2015, to review existing and emerging opportunities for international collaboration and evaluate their technical merit and cost/benefit ratio, to align these opportunities with the current and planned work scope within UFD work packages for possible leveraging, and to develop a revised portfolio of international R&D activities that align with goals, priorities, and funded plans of the UFD program. As a result of this process, UFD decided in FY15 to end its participation in the CFM Project because of its relatively narrow focus and relatively high participatory cost.

Another discussion point is whether DOE/UFD can and should move from a mostly participatory role in ongoing URL experiments conducted by other nations, to a more active role in developing its own experimental program specifically tailored to the DOE/UFD needs. Some collaborative initiatives like the Mont Terri Project definitely provide the opportunity to involve partners, such as DOE, to conduct their own experimental work. As mentioned earlier in this document, other international partners can be found if the proposed work aligns well with the interests of other Mont Terri organizations. It is important to note in this context that the existing infrastructure at Mont Terri makes developing and conducting experiments very easy, even if the proposing partner is located far away from the URL. Swisstopo can handle a lot of the organizational details if needed, and there is a long list of experienced contractors that are available to conduct the actual experimental work. There are currently no immediate plans for DOE to move into a more active role conducting its own experiments at URLs of opportunity. However, because of DOE's interest in the feasibility of direct geological disposal of large spent nuclear fuel canisters currently in dry storage (Hardin et al., 2014), the important question arises whether clay-based barriers can withstand temperatures higher than the 100 °C threshold for bentonite performance usually assumed in advanced repository designs. In the future, there could be a need for a targeted high-temperature heater experiment developed or co-developed by DOE, which could be done in, for example, at Mont Terri or the Grimsel Test Site (see Section 3.3.3.2).

Table 5-1. Summary and Ranking of International Programs in Cooperative Initiatives Related to URLs: Status as of September 2014. The FEPs ranking is based on Tables 7 and 8 in Nutt (2011). Table entries are sorted by URLs.

URL	Relevant Ongoing or Planned Experiments (Selected)	Cooperation Mode	Main Focus	FEPs Ranking based on Tables 7 and 8 in Nutt (2011)	Test Period
Mont Terri, Switzerland (Opalinus Clay)	FE: Full-scale heater test demonstration experiment	Via Mont Terri Project	Both EBS and NBS NBS: Many aspects of near-field shale repository evolution, such as EDZ creation, desaturation and resaturation, thermal effects, pore-pressure increase after backfilling and heating EBS: Performance of EBS backfilling and lining technology	Geosphere FEPS (for shale): 2.2.01: Excavation Disturbed Zone (EDZ) >> High (Shale) 2.2.07: Mechanical Processes >> Medium (Shale) 2.2.08: Hydrologic Processes >> Medium (Shale) 2.2.11: Thermal Processes >> Medium (Shale) Engineered System FEPS: Buffer/Backfill materials 2.1.04.01: Buffer/Backfill >> High 2.1.07.02, .03., .04., .09: Mechanical Processes >> Medium 2.1.08.03, .07, .08: Hydrological Processes >> Medium 2.1.11.04: Thermal Processes >> Medium Engineered System FEPS: Seal/liner materials 2.1.05.01: Seals >> Medium 2.1.07.02, .08., .09: Mechanical Processes >> Medium 2.1.08.04, .05, .07, .08, .09: Hydrological Processes >> Low	Heating started in early 2015
Mont Terri, Switzerland	HE-E: Half-scale heater test in VE test section (VE = Ventilation Experiment)	Via DECOVALEX Project	Mostly EBS EBS: Non-isothermal resaturation behavior in bentonite backfill NBS: Interaction of near-field shale rock with EBS components	Geosphere (for shale): 2.2.01: Excavation Disturbed Zone (EDZ) >> High (Shale) 2.2.07: Mechanical Processes >> Medium (Shale) 2.2.08: Hydrologic Processes >> Medium (Shale) 2.2.11: Thermal Processes >> Medium (Shale) 2.2.09: Chemical Processes – Transport >> Medium-High Engineered System FEPS: Buffer/Backfill materials 2.1.04.01: Buffer/Backfill >> High 2.1.07.02, .03., .04., .09: Mechanical Processes >> Medium 2.1.08.03, .07, .08: Hydrological Processes >> Medium 2.1.11.04: Thermal Processes >> Medium	Heating phase: June 2011 through 2018
Mont Terri, Switzerland	MB: Mine-by Test for full-scale HM validation	Via Mont Terri Project	NBS Excavation-generated response in the argillaceous clay host rock near a mined tunnel, including changes in the near-field hydrologic properties	Geosphere FEPS (for shale): 2.2.01: Excavation Disturbed Zone (EDZ) >> High (Shale) 2.2.07: Mechanical Processes >> Medium (Shale) 2.2.08: Hydrologic Processes >> Medium (Shale)	2008 – 2009

URL	Relevant Ongoing or Planned Experiments (Selected)	Cooperation Mode	Main Focus	FEPs Ranking based on Tables 7 and 8 in Nutt (2011)	Test Period
Mont Terri, Switzerland	HG-A: Gas path host rock and seals	Via Mont Terri Project	Mostly NBS Investigation of EDZ as preferential flow path for gases generated from corrosion	Geosphere FEPS (for shale): 2.2.01: Excavation Disturbed Zone (EDZ) >> High (Shale) 2.2.08: Hydrologic Processes >> Medium (Shale) 2.2.12: Gas sources and effects >> Low	Ongoing since 2006 in various stages with hydraulic and gas injection tests
Mont Terri, Switzerland	DR-A: Diffusion, retention and perturbations	Via Mont Terri Project	NBS Long-term diffusion behavior of sorbing and non-sorbing radionuclides in clay	Geosphere FEPS (for shale) 2.2.05: Flow and Transport Pathways >> Medium (Shale) 2.2.08: Hydrologic Processes >> Medium (Shale) 2.2.09: Chemical Processes – Transport >> Medium (Shale)	2011 – 2013
Grimsel Test Site, Switzerland	CFM: RN tracer test	Via CFM Project	NBS Transport behavior of a tracer/radionuclide “cocktail” in a shear zone. Test includes conservative tracers, weakly sorbing solutes, strongly sorbing solutes and bentonite colloids	Geosphere FEPS (for crystalline rock) 2.2.05: Flow and Transport Pathways >> Medium (Crystalline) 2.2.08: Hydrologic Processes >> Low (Crystalline) 2.2.09: Chemical Processes – Transport >> Medium (Crystalline)	Several tests in 2009 through 2012
Grimsel Test Site, Switzerland	CFM: RN-Doped Plug Experiment	Via CFM Project	NBS: Similar to above test, but this time involving at radionuclide-doped bentonite plug which erodes and induces colloid-facilitated transport	Geosphere FEPS (for crystalline rock) 2.2.05: Flow and Transport Pathways >> Medium (Crystalline) 2.2.08: Hydrologic Processes >> Low (Crystalline) 2.2.09: Chemical Processes – Transport >> Medium (Crystalline) Engineered System FEPS: Buffer/backfill materials 2.1.04.01: Buffer/Backfill >> High 2.1.09.51-59, .61: Chemical Processes –Transport >> Low to Medium	Started in May 2014
Grimsel Test Site, Switzerland	FEBEX-DP: Full-scale heater test dismantling project	Via FEBEX-DP Project	Mostly EBS Long-term performance of the bentonite backfill and, to a lesser degree, the near-field crystalline rock, with emphasis on the thermal evolution and resaturation of bentonite backfill surrounding a heated waste package	Engineered System FEPS: Buffer/Backfill materials 2.1.04.01: Buffer/Backfill >> High 2.1.07.02, .03., .04., .09: Mechanical Processes >> Medium 2.1.08.03, .07, .08: Hydrological Processes >> Medium 2.1.11.04: Thermal Processes >> Medium Geosphere FEPS (for crystalline rock) 2.2.01: Excavation Disturbed Zone (EDZ) >> Medium (Crystalline) 2.2.07: Mechanical Processes >> Low (Crystalline) 2.2.08: Hydrologic Processes >> Low (Crystalline) 2.2.11: Thermal Processes >> Low (Crystalline)	Heater test ongoing since 1997; dismantling conducted in Summer 2015

URL	Relevant Ongoing or Planned Experiments (Selected)	Cooperation Mode	Main Focus	FEPs Ranking based on Tables 7 and 8 in Nutt (2011)	Test Period
Grimsel Test Site, Switzerland	GAST: Gas permeable seal experiment	Possibly via MoU with NAGRA	EBS Demonstrate the performance of repository seals and to improve the understanding of water and gas transport through these sealing systems. The experiment involves specially designed backfill and sealing materials such as high porosity mortars or sand/bentonite (S/B) mixtures.	Engineered System FEPS: Buffer/Backfill materials 2.1.04.01: Buffer/Backfill >> High 2.1.08.03, .07, .08: Hydrological Processes >> Medium 2.1.12.01, .02, .03: Gas sources and effects >> Medium	2010 – 2015
Äspö Hard Rock Laboratory, Sweden	BRIE: Bentonite rock interaction experiment	Via SKB Task Forces	Both NBS and EBS Understand the exchange of water and potential bentonite erosion at the interface between backfill and flowing fractures	Engineered System FEPS: Buffer/Backfill materials 2.1.04.01: Buffer/Backfill >> High 2.1.08.03, .07, .08: Hydrological Processes >> Medium Geosphere FEPS (for crystalline rock) 2.2.05: Flow and Transport Pathways >> Medium (Crystalline) 2.2.08: Hydrologic Processes >>Low (Crystalline)	Ongoing since 2012
Äspö Hard Rock Laboratory, Sweden	LTDE-SD: Long-term sorption diffusion experiment	Via SKB Task Forces	NBS Diffusion and sorption in a conducting fracture and adjacent matrix (sorbing and non-sorbing tracers)	Geosphere FEPS (for crystalline rock) 2.2.05: Flow and Transport Pathways >> Medium (Crystalline) 2.2.08: Hydrologic Processes >>Low (Crystalline) 2.2.09: Chemical Processes – Transport >> Medium (Crystalline)	Completed in 2010 with 6 months test duration
Äspö Hard Rock Laboratory, Sweden	Prototype Repository: full-scale prototype tunnels with six deposition holes	Via SKB Task Forces	Mostly EBS, also NBS Demonstration of the integrated function of the repository and a full-scale reference for test of predictive models concerning individual components as well as the complete repository system. Includes heaters and backfill.	Geosphere FEPS (for shale): 2.2.01: Excavation Disturbed Zone (EDZ) >> High (Shale) 2.2.07: Mechanical Processes >> Medium (Shale) 2.2.08: Hydrologic Processes >> Medium (Shale) 2.2.11: Thermal Processes >> Medium (Shale) Engineered System FEPS: Buffer/Backfill materials 2.1.04.01: Buffer/Backfill >> High 2.1.07.02, .03., .04., .09: Mechanical Processes >> Medium 2.1.08.03, .07, .08: Hydrological Processes >> Medium 2.1.11.04: Thermal Processes >> Medium	Since 2001. Outer test section opened and retrieved in 2011.

URL	Relevant Ongoing or Planned Experiments (Selected)	Cooperation Mode	Main Focus	FEPs Ranking based on Tables 7 and 8 in Nutt (2011)	Test Period
Tournemire, France	SEALEX: Long-time sealing experiment for different materials	Via DECOVALEX	Mostly EBS Long-term isothermal HM© behavior and hydraulic performance of swelling clay-based seals	Engineered System FEPS: Seal/liner materials 2.1.05.01: Buffer/Backfill >> Medium 2.1.07.02, .08., .09: Mechanical Processes >> Medium 2.1.08.04, .05, .07, .08, .09: Hydrological Processes >> Medium (Flow through seals) 2.1.09.01, .03, .09, .13: Chemical Processes – Chemistry >> Medium	2011 – 2015
Bedrichov Tunnel, Czech Republic	Flow patterns and tracer transport in fractured granite	Via DECOVALEX	NBS Flow patterns and tracer transport behavior within fractured crystalline rock	Geosphere (for crystalline rock): 2.2.02: Host Rock Properties >> High (Crystalline) 2.2.05: Flow and Transport Pathways >> Medium (crystalline) 2.2.08: Hydrologic Processes >> Medium (Crystalline)	Hydrogeologic characterization and monitoring ongoing
Horonobe URL, Japan	EBS experiment: Vertical heater and buffer test (planned)	Via DECOVALEX	Mostly EBS EBS: Non-isothermal resaturation behavior in bentonite backfill NBS: Interaction of near-field shale rock with EBS components	Geosphere (for shale): 2.2.01: Excavation Disturbed Zone (EDZ) >> High (Shale) 2.2.07: Mechanical Processes >> Medium (Shale) 2.2.08: Hydrologic Processes >> Medium (Shale) 2.2.11: Thermal Processes >> Medium (Shale) Engineered System FEPS: Buffer/Backfill materials 2.1.04.01: Buffer/Backfill >> High 2.1.07.02, .03., .04., .09: Mechanical Processes >> Medium 2.1.08.03, .07, .08: Hydrological Processes >> Medium 2.1.11.04: Thermal Processes >> Medium	Start of heating phase in late 2014
KURT URL, Korea	Streaming potential (SP) testing and correlation with groundwater flow	Via MoU with KAERI	NBS: Flow patterns in fractured crystalline rock	Geosphere (for crystalline rock): 2.2.02: Host Rock Properties >> High (Crystalline) 2.2.05: Flow and Transport Pathways >> Medium (crystalline) 2.2.08: Hydrologic Processes >> Medium (Crystalline)	*In situ* testing will be conducted once the KURT extension is complete
KURT URL, Korea	Development of techniques for *in situ* borehole characterization and monitoring	Via MoU with KAERI	NBS: Relevance to deep borehole disposal	Geosphere FEPS (for borehole): 2.2.01: Excavation Disturbed Zone (EDZ) >> High (Borehole) 2.2.07: Mechanical Processes >> Low (Borehole) 2.2.08: Hydrologic Processes >> Medium (Borehole) 2.2.11: Thermal Processes >> Medium (Borehole) 2.2.09: Chemical Processes – Chemistry >> Medium-High (Borehole) 2.2.09: Chemical Processes – Transport >> Medium-High (Borehole) 2.2.02: Host Rock (properties) >> High (Borehole) 2.2.05. Flow and Transport Pathways >> Medium (Borehole)	Ongoing

URL	Relevant Ongoing or Planned Experiments (Selected)	Cooperation Mode	Main Focus	FEPs Ranking based on Tables 7 and 8 in Nutt (2011)	Test Period
HADES URL, Belgium	PRACLAY: Full-scale seal and heater experiment	Possibly via bilateral collaboration with SCK/CEN	Mostly NBS Many aspects of near-field boom clay repository evolution, such as EDZ creation, desaturation and resaturation, thermal effects, pore-pressure increase after backfilling and heating	Geosphere FEPS (for shale): 2.2.01: Excavation Disturbed Zone (EDZ) >> High (Shale) 2.2.07: Mechanical Processes >> Medium (Shale) 2.2.08: Hydrologic Processes >> Medium (Shale) 2.2.11: Thermal Processes >> Medium (Shale)	Heating started January 2015
HADES URL, Belgium	RN Migration: Long-running RN diffusion tests	Possibly via bilateral collaboration with SCK/CEN	NBS Diffusion-controlled migration of radionuclides in clay rocks	Geosphere FEPS (for shale) 2.2.05: Flow and Transport Pathways >> Medium (Shale) 2.2.09: Chemical Processes – Transport >> Medium (Shale)	Ongoing since more than two decades

Table 5-2. Current and Future Work Package Activities with International Collaboration and Focus on URL Experiments (sorted by URL)

URL	Relevant Ongoing or Planned Experiments (Selected)	Cooperation Mode	UFD Participation
Mont Terri, Switzerland (Opalinus Clay)	• FE: Full-scale heater test demonstration experiment • HE-E: Half-scale heater test in VE test section • HG-A: Gas path host rock and seals • DR-A: Diffusion, retention and perturbations • EB: Engineered Barrier Experiment FS: Fault Slip Experiment	• Mont Terri Project • DECOVALEX-2015 • Mont Terri Project • Mont Terri Project • DECOVALEX-2019 • DECOVALEX-2019	• LBNL • LBNL • LBNL (Complete) • LBNL (Complete) • Maybe • Maybe
Grimsel Test Site, Switzerland (Granite)	• CFM: RN tracer test and RN-doped plug experiment • FEBEX-DP: full-scale heater test dismantling	• CFM • FEBEX-DP	• LANL, LLNL (Complete) • SNL, LANL, LBNL
Äspö Hard Rock Laboratory, Sweden (Granite)	• BRIE: Bentonite rock interaction experiment • LTDE-SD and REPRO (Diffusion-Advection-Sorption) • LASGIT	• SKB Task Forces • SKB Task Forces • DECOVALEX-2019	• LANL (Complete) • Likely, LANL • Maybe
Mizunami, Japan (Granite)	• GREET: Groundwater Recovery Experiment	• DECOVALEX-2019	• Maybe
Bedrichov Tunnel, Czech Republic (Granite)	• Flow patterns and tracer transport in fractured granite	• DECOVALEX-2015	• Ongoing, SNL
Horonobe URL, Japan (Sedimentary rock)	• EBS experiment: Vertical heater and buffer test (planned)	• DECOVALEX-2015	• Ongoing, LBNL
KURT URL, Korea (Crystalline rock)	• Streaming potential (SP) testing regarding correlation with groundwater flow • Technique development for *in situ* borehole characterization	• MoU KAERI • MoU KAERI	• Ongoing, SNL • Ongoing, SNL
LSMHM URL, France (COX Clay)	• Alveole Heater Test	• DECOVALEX-2019 (Tentative)	• Maybe

6. STATUS OF INTERNATIONAL COLLABORATION ACTIVITIES WITH FOCUS ON URL EXPERIMENTS

Here we give a brief description of ongoing international collaboration activities involving UFD scientists. The section is dedicated to R&D work with primary focus on participation in, and analysis of, URL experiments, as described in Table 5-2. We start with research work addressing issues related to near-field perturbation and engineered barrier integrity (Section 6.1), followed by R&D understanding fluid flow and radionuclide transport processes in the host rock (Section 6.2), and end with collaborative research to develop new characterization and monitoring methods (Section 6.3). Example R&D results will be presented, albeit without providing exhaustive explanations; we intend to merely illustrate technical achievements made in various areas. All necessary detail can be found in the references given throughout the text. International collaboration activities unrelated to URLs are briefly described in Section 7.

6.1 Near-Field Perturbation and EBS Integrity

6.1.1 THM Modeling of Heater Experiments

On behalf of DOE, LBNL has been participating in the DECOVALEX-2015 Project since 2012 as one of the international modeling teams working on Task B1, the HE-E Heater Test at Mont Terri (Section 3.1.4) and Task B2, the Horonobe Engineered Barrier Experiment (Section 3.1.5). LBNL has also been contributing to the design and scoping simulations for the FE Heater Test at Mont Terri. As described in Section 4 of the milestone report entitled "*Investigation of Coupled Processes and Impact of High Temperature Limits in Argillite Rock*," FCRD-UFD-2015-000362, (Zheng et al., 2015), the TOUGH-FLAC simulator developed at LBNL is the primary analysis tool, because this simulator has the required capabilities to model a large variety of problems associated with nuclear waste disposal for various engineering and natural systems. TOUGH-FLAC can simulate coupled THM processes under multiphase flow conditions through a sequential coupling of the TOUGH2 multiphase flow simulator with the FLAC3D geomechanical code (Rutqvist et al., 2002; Rutqvist, 2011). As part of the UFD R&D program, TOUGH-FLAC has been modified for applications related to bentonite-backfilled repositories in clay host formations (Rutqvist et al., 2014a). Major improvements include implementation of the Barcelona Basic Model (BBM) for the rigorous THM modeling of behavior of swelling soils and applied to modeling of bentonite backfill behavior (Alonso et al., 1990). The BBM model can describe many typical features of unsaturated-soil mechanical behavior, including wetting-induced swelling or collapse strains, depending on the magnitude of applied stress, as well as the increase in shear strength and apparent preconsolidation stress with suction (Gens et al., 2006).

Recently, the BBM has been extended to a dual-structure model, referred to as the Barcelona Expansive Model (BExM). In a dual-structure model, the material consists of two structural levels: a microstructure in which the interactions occur at the particle level, and a macrostructure that accounts for the overall fabric arrangement of the material comprising aggregates and macropores (Gens et al., 2006, Sánchez et al., 2005). A dual-structure model has important features for modeling the mechanical behavior of a bentonite buffer, such as irreversible strain during suction cycles. However, most importantly, a dual-structure model provides the necessary link between chemistry and mechanics, enabling us to develop a coupled THMC model for the analysis of long-term EBS behavior. This approach enables mechanistic modeling of processes important for long-term buffer stability, including effects of pore-water salinity on swelling (loss of swelling), conversion of smectite to nonexpansive mineral forms (loss of swelling), and swelling pressure versus exchangeable cations (Rutqvist et al. 2014b).

6.1.1.1 Status of Participation in DECOVALEX Task B1

Eight international modeling teams are participating in Task B1 of DECOVALEX-2015. Instead of starting directly with the interpretation and simulation of the rather complex HE-E heater experiment, Task B1 included several modeling steps of increasing complexity: (1) the study of THM processes in the host rock, using data from an earlier borehole heater test (HE-D experiment); (2) the study of THM processes in the buffer materials, using data from laboratory experiments (CIEMAT Column Experiments), and (3) the study of the ongoing HE-E experiment considering the host rock as well as the buffer material, initially as a predictive exercise, then as an interpretative effort with comparison to monitoring data (Garitte and Gens, 2012). Regarding the HE-E experiment, the main objective is to test model capabilities addressing the evolution of EBS components and the near-field Opalinus Clay in the early post-closure perturbation period, with emphasis on thermal evolution, resaturation, and evolution of swelling pressure in bentonite backfill.

The first step of modeling the HE-D experiment started in 2012 and was completed in November 2013. LBNL's modeling of the HE-D experiment and comparison of the TOUGH-FLAC modeling results to those of other DECOVALEX modeling teams were reported in the FY2013 milestone report entitled "*THM and Reactive Transport Model Development and Evaluation: International Activities,*" FCRD-UFD-2013-000372 (Rutqvist et al., 2013). Simulating the THM behavior in this test allowed initial model comparison and validation without the complicating THM interaction with engineered barrier components. The second step, a study of bentonite properties through modeling of laboratory experiments, were completed in FY14 and described in the FY14 milestone report entitled "*Investigation of Coupled Processes and Impact of High Temperature Limits in Argillite Rock*," FCRD-UFD-2014-000493 (Zheng et al., 2014). The predictive and finally interpretive modeling of the HE-E experiment (the final step of Task B1) is ongoing; details on the current modeling status and model comparison results are given in Zheng et al., 2015). Below, we provide brief descriptions of the LBNL modeling studies conducted for the HE-D heater test, the CIEMAT column experiments, and for the HE-E experiment.

The HE-D experiment was conducted at the Mont Terri URL between March 2004 and June 2005 by heating of Opalinus Clay from two heaters placed in a horizontal borehole (Wileveau, 2005; Gens et al., 2007). About 30 temperature sensors, 10 water pressure sensors, and 3 extensometers were placed around this heating borehole (Figure 6-1). Approximately one month after installation, the heaters were switched on with a total power of 650 W (325 W per heater). The heaters were then maintained under constant power for 90 days. Afterwards, the power was increased threefold, to 1950 W (975 W per heater), and maintained at that level for a further 248 days. At the end of this second heating stage, the heaters were switched off and the clay was allowed to cool down. Temperature, pore pressure, and deformation were measured throughout.

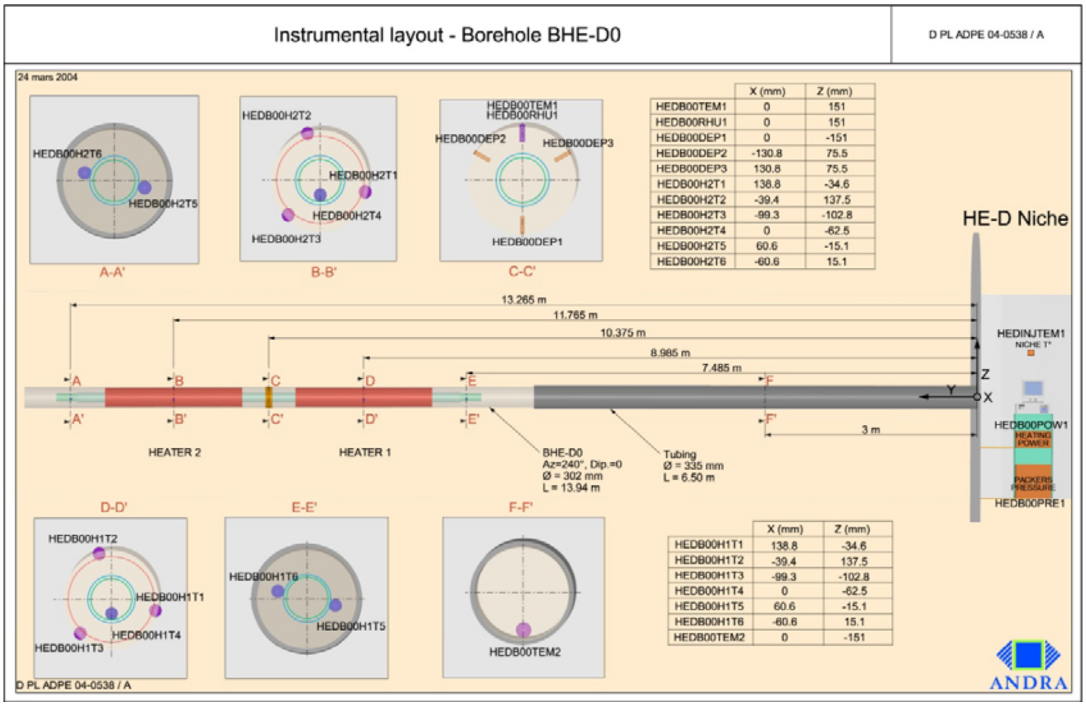


Figure 6-1. Layout of the heater borehole of the HE-D Heater Test at Mont Terri URL (from Garitte and Gens, 2012)

LBNL modeled the HE-D experiment using the TOUGH-FLAC simulator. Anisotropic material models were employed to account for the effect of sedimentation planes found in the Opalinus Clay. Figure 6-2 shows typical simulation results at two temperature monitoring points near the heaters, and one strain gage at another location in the perturbed rock mass. The simulation shows a correlation between temperature and fluid pressure as a result of thermal pressurization, which is caused by the differences in the coefficient of thermal expansion between the fluid and the solid rock. Temperature is in good agreement with measured data when an anisotropic thermal conductivity is used. Simulated pressure and strain are also in reasonable agreement with the measurements. The radial strain indicates mainly compression during heating as rock is expanded from the heated borehole.

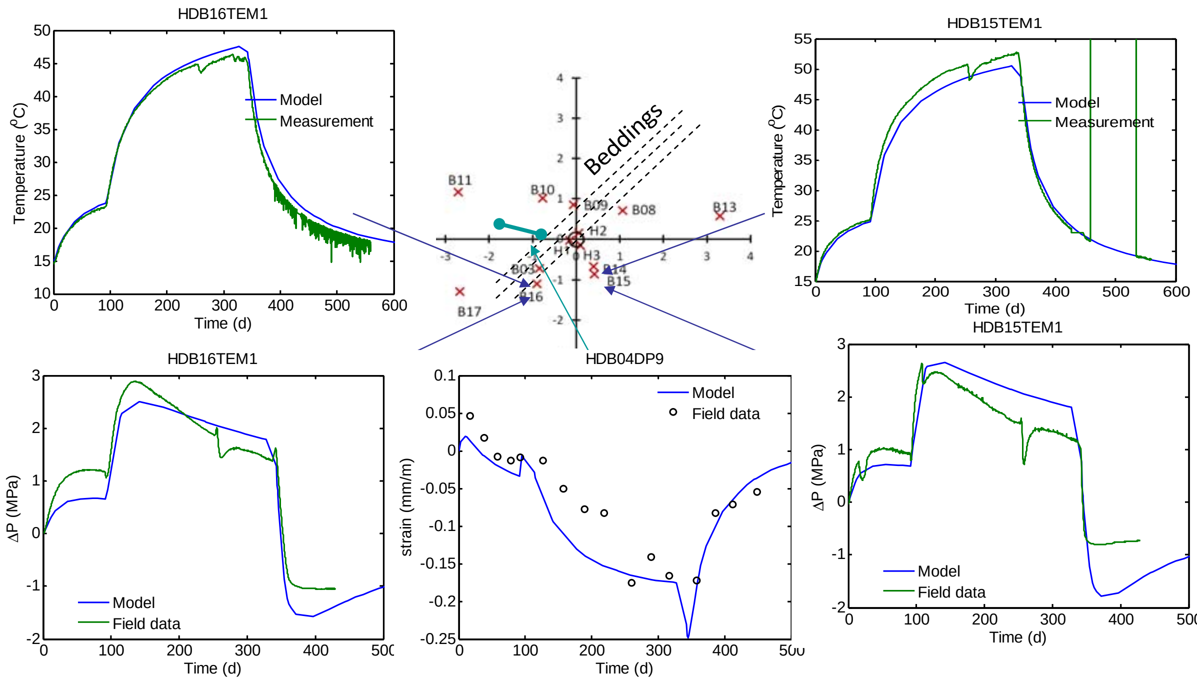


Figure 6-2. Comparison of simulated and measured temperature and pressure at two monitoring points (B15 and B16) and strain at another location close to the heater (from Rutqvist et al., 2013)

Figure 6-3 gives a comparison of simulation results obtained by the eight teams involved in modeling the HE-D experiment of DECOVALEX-2015 with the measured data by two temperature sensors located, respectively, at a distance of 1.11 m away from the center of the heater parallel to bedding (HEDB03), and at a distance of 0.775 m away from the center of the heater perpendicular to bedding (HEDB14). Despite the different distances to the heater, both sensors show a similar course of temperature evolution over time, which illustrates the effect of anisotropic heat conduction in the Opalinus Clay. Overall, the figure demonstrates good agreement between the results of the different groups. Furthermore, the temperature observations are well enveloped by the modeling results of the eight teams. The largest disagreement is observed at sensor HEDB14, where the simulated temperature is strongly overestimated by one of the international modeling teams. This particular simulation was conducted with an axisymmetric model in which thermal anisotropy cannot be considered. The comparative evaluation shown in Figure 6-3 is a good example of the value that DECOVALEX-type model comparison studies can provide to system understanding and model validation. The fact that several individual research groups with their own simulation tools and conceptual understanding arrive at similar model predictions enhances confidence in the robustness of THM models. And the possibility of linking model differences to particular choices in conceptual model setup provides guidance into "best" modeling choices and understanding the effect of conceptual model variability.

The CIEMAT column experiments tested the thermal hydration behavior in two buffer materials, granular bentonite (or bentonite pellets) and a sand/bentonite mixture (Figure 6-4). The design of the column experiments mimicked the HE-E conditions, with the height of the column equal to the thickness of the buffer filled between the canister and the host rock. A heater was placed at the bottom and a cooler at the top of each column, so that the column was heated while the top remained at an ambient temperature of ~21.5°C. Sensors were installed at distances of 10 cm, 22 cm, and 40 cm from the heater to measure temperature and relative humidity. The experiment was conducted in several stages with changing boundary/heating conditions, as illustrated in Figure 6-4. The simulation objective was to predict the transient fluid-flow and heat-transfer processes that occur in the experiment, and to calibrate the evolution of flow and thermal properties of the two hydrating buffer materials against the experimental measurements.

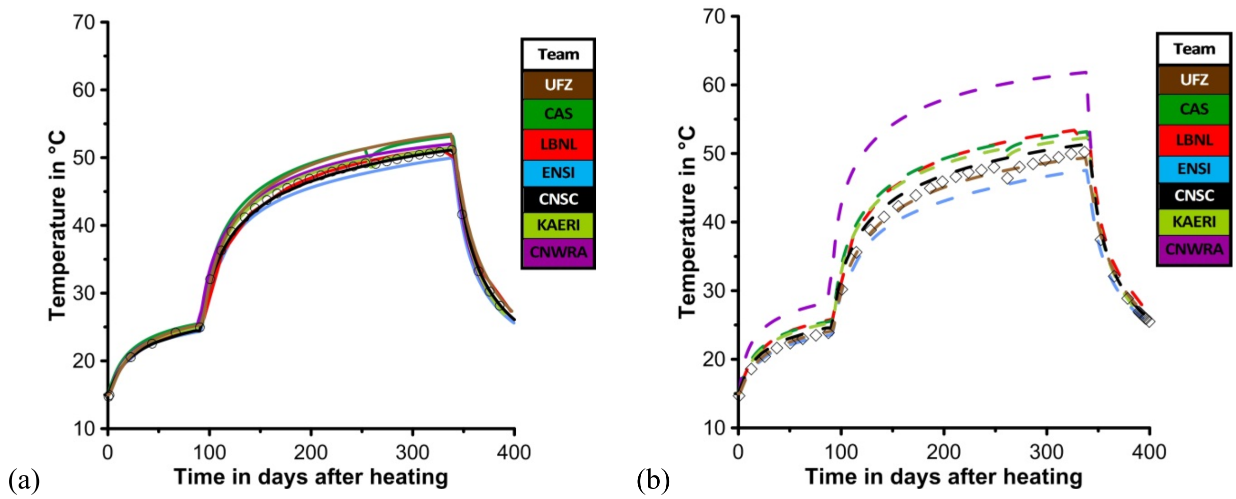


Figure 6-3. Comparison of measurements and model results of for the temperature evolution over time at sensors HEDB03 (a) and HEDB14 (b) (from Graupner et al., 2013)

Figure 6-5 shows selected simulation results after model calibration by the LBNL team. After heating is initiated, the temperature at the 10 cm location increases rapidly to ~30°C. Further step-wise increases occur when the insulation is changed and later as the heater temperature is raised to 140°C. The simulated relative humidity at 10 cm also increases rapidly after heating starts, due to the increase in temperature and the vapor flowing up from the bottom. There are complex couplings at play. When temperature increases at the 10 cm location, the relative humidity becomes larger as the capillary pressure drops, even if the water saturation remains unchanged. However, heating also causes the vapor pressure to increase near the heater, which drives vapor flowing up and contributes to the increased relative humidity at the 10 cm location during the early stage of heating. Over time, the relative humidity decreases at the 10 cm location. This is because further heating causes the drying at the 10 cm location with the vapor flowing further up. This upflow of vapor is evidenced by the continuous increase in relative humidity at the 22 cm and 40 cm locations, which in part is also caused by as a result of liquid water flowing downward from the top of the cell via gravity and capillary forces. Overall, the simulated temperatures and relative humidity values at three locations are in a good agreement with the measured ones.

The simulations for the CIEMAT column experiments demonstrate the complexity of the coupled processes involved in the temperature and hydration behavior of heated bentonite. Results also indicate the importance of adequately understanding experimental boundary conditions, such as the water intake of the experimental column or the substantial heat loss from the equipment that has to be considered in order to characterize the thermal properties of the buffer material. Modeling teams learned that one can obtain a unique solution for back-calculating the thermal and hydraulic properties of the buffer material by evaluating the transient temperature and moisture responses in addition to steady-state profiles. By accounting for the enhanced permeability of gas and the temperature dependency of the capillary pressure, the models can reasonably reproduce the evolution of relative humidity along the column in the experiments.

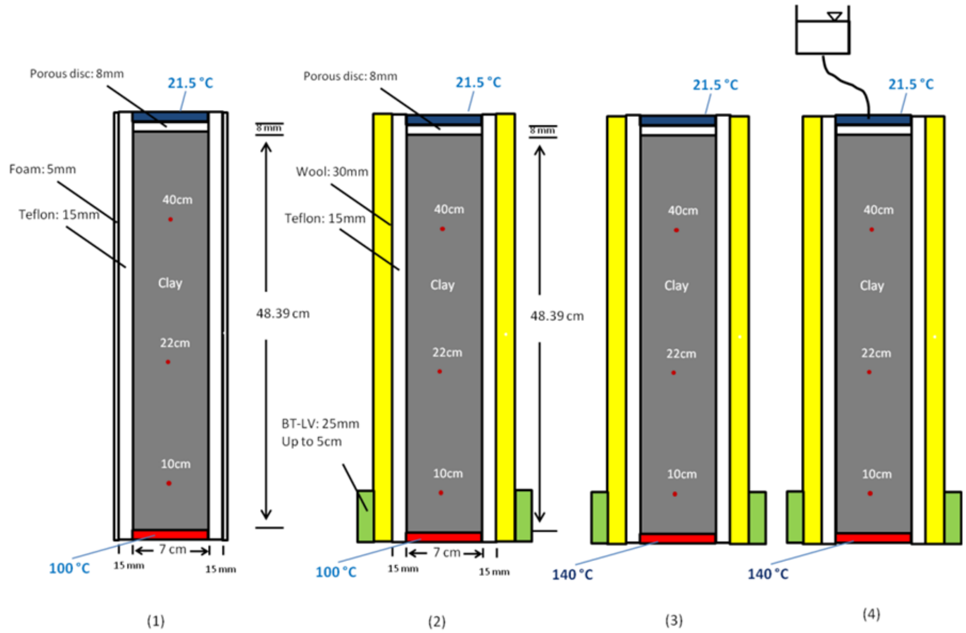


Figure 6-4. Schematic of experimental setups of column experiment in sequential steps: (1) Heating at temperature of 100 ˚C from 0 to 1566 hours, (2) heating with new insulation layer from 1566 to 3527 hours, (3) heating at 140 ˚C from 3527 to 5015 hours, (4) heating with hydration valve open after 5015 hours (from Zheng et al., 2014)

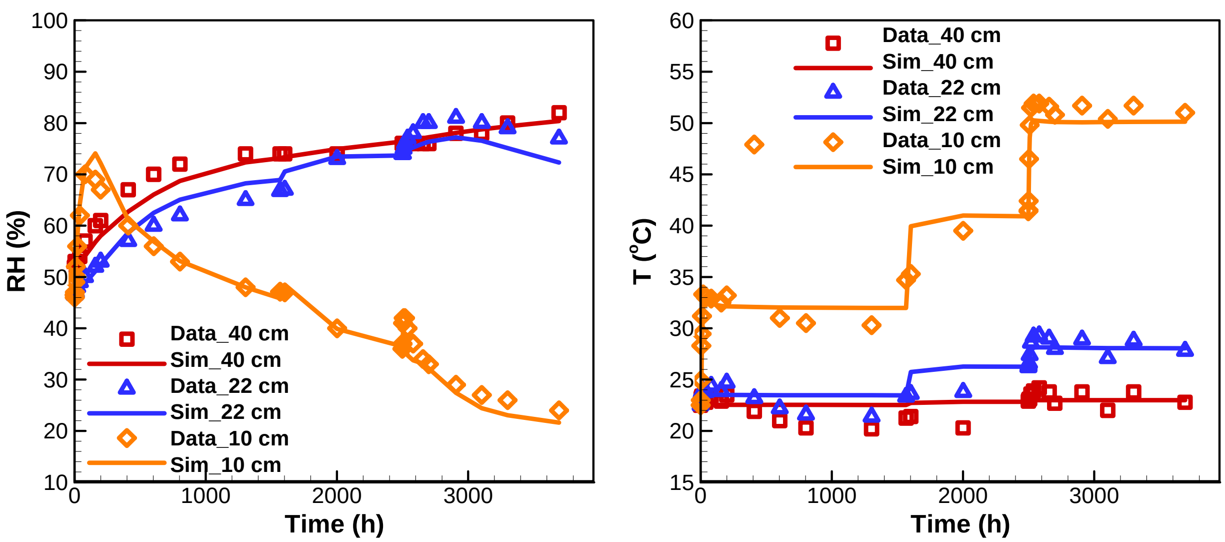


Figure 6-5. Simulated and measured relative humidity (RH) and temperature (T) as a function of time after heater was turned on (from Zheng et al., 2014)

As described in Section 3.1.2.2, the Mont Terri HE-E Experiment focuses on the THM behavior of bentonite barriers in the early nonisothermal resaturation stage and their THM interaction with Opalinus Clay. The objective is to better understand the evolution of a disposal system for high level waste in the early post-closure period, with emphasis on the thermal evolution, buffer resaturation (in situ determination of the thermal conductivity of bentonite and its dependency on saturation), pore-water pressure in the near field, and the evolution of swelling pressures in the buffer (Gaus et al., 2014). Similar to other modeling teams involved in this DECOVALEX task, LBNL first conducted a predictive analysis of the HE-E experiment, before the field data were available to the DECOVALEX-2015 participants, followed by a comparison of the initial model predictions with experimental results. A final interpretive modeling of the field experimental data and comparison with other modeling teams is ongoing and will be completed during the rest of calendar year 2015.

Figure 6-6 shows LBNL's 3-D model grid for the HE-E experiment and its location within the Mont Terri URL. It is a half symmetric model with a vertical symmetry plane along the tunnel axis. In the model, the relevant materials are represented, including the different types of bentonite materials. The most important thermal and hydraulic properties were derived from literature data and from material properties estimated by modeling of various THM laboratory experiments on bentonite.

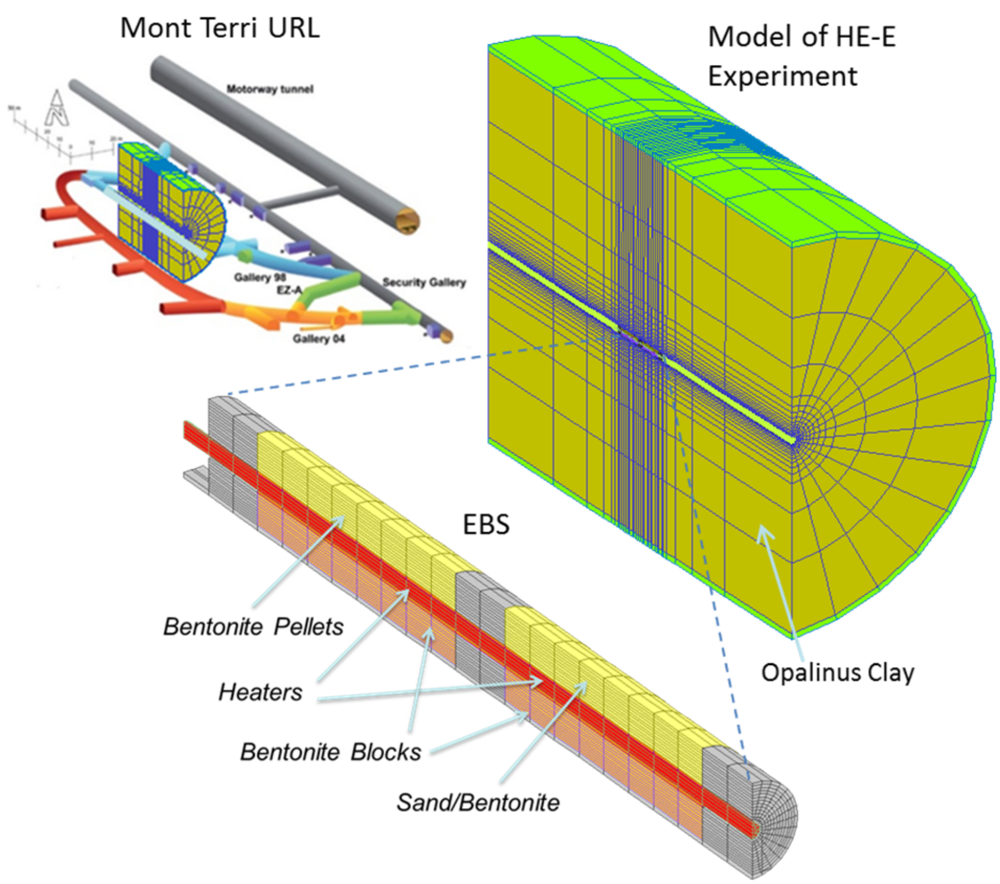


Figure 6-6. TOUGH-FLAC 3-D model of the Mont Terri HE-E experiment (from Zheng et al., 2015)

A comparison of the predicted and observed evolutions of relative humidity and temperature is shown in Figure 6-7. The figure shows that the general humidity behavior of the bentonite at the rock wall and drying of the inner parts of the bentonite buffer is captured well in the modeling. Model results for relative humidity, which is related to saturation, show very good agreement with measurements for the blue and red curves (i.e. close the rock wall and close to the heater). However, the model overestimates relative humidity in the mid part of the bentonite buffer (green curve). A parameter study was performed as to identify possible reasons for this discrepancy in the wetting of the bentonite buffer. The included variation of buffer absolute permeability (no significant effect), diffusion coefficient (did not help) and buffer relative permeability (tried to reduce relative permeability, but this did not help). A possible reason that will be investigated next is the high suction part of the water retention curve with the van-Genuchten water retention model may cause important deviations from the experimental data at low saturation. Nevertheless, the overall evolution of relative humidity was reasonably predicted by the modeling.

Figure 6-8 shows the evolution of fluid pressure within Opalinus Clay at a monitoring point located 3.54 m from the tunnel wall. This increase in fluid pressure is a result of so-called thermal pressurization, caused by thermal expansion of the pore fluid that cannot escape in the relatively low-permeability host rock. The magnitude and duration of this excess pressure pulse depends on parameters such as rock permeability, and compressibility of water and rock. Using the Opalinus Clay properties determined from the modeling of the HE-D experiments, it appears that the model can predict this pressure increase fairly well.

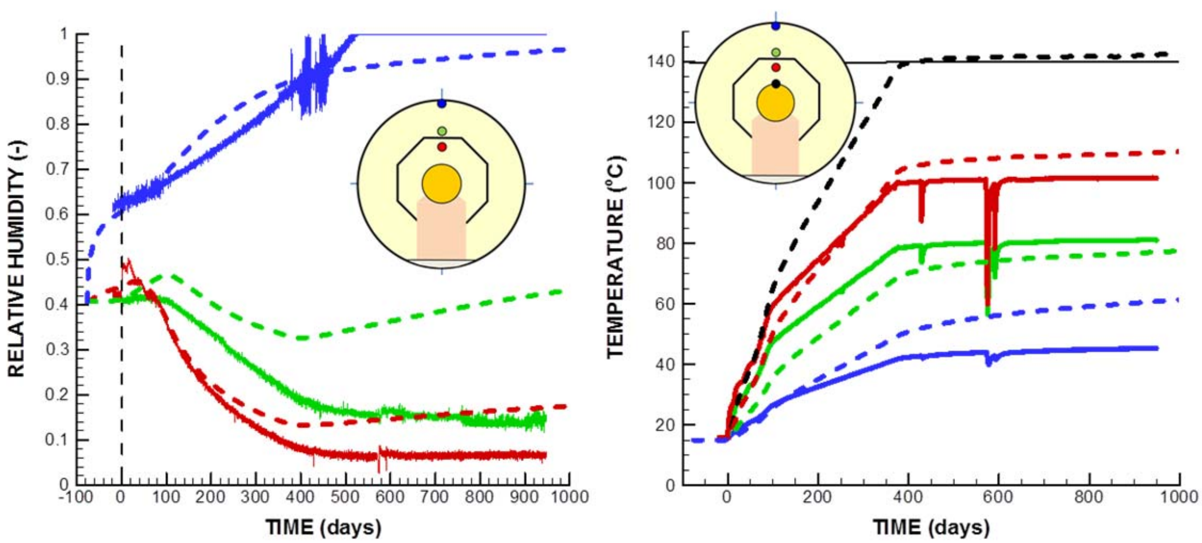


Figure 6-7. Comparison of predicted (dashed lines) and measured (solid lines) evolutions of (a) relative humidity and (b) temperature, in a cross section of the HE-E experiment (from Zheng et al., 2015)

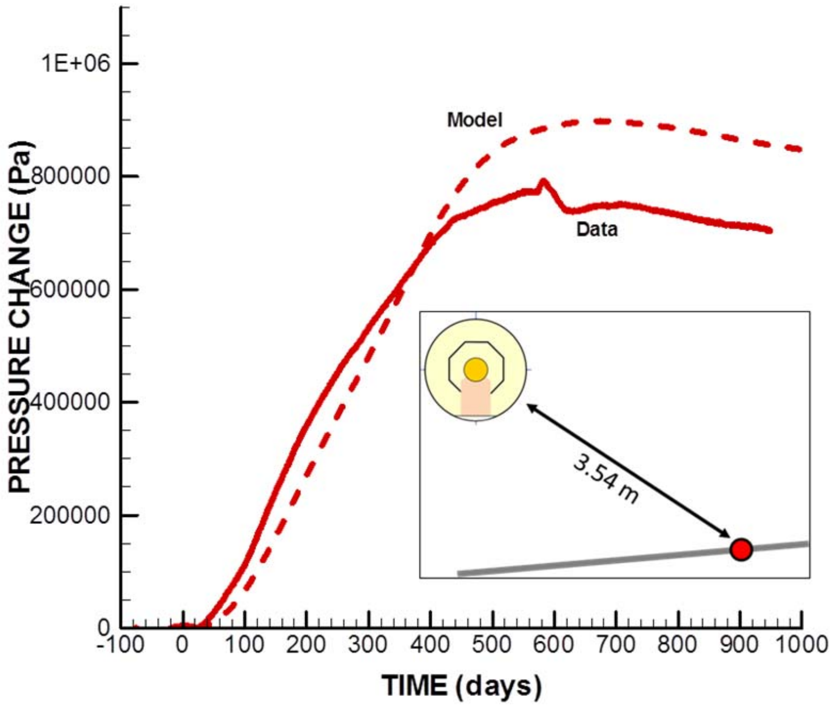


Figure 6-8. Comparison of predicted (dashed lines) and measured (solid lines) evolutions of pore pressure in Opalinus Clay at a point located 3.54 m from the tunnel wall (from Zheng et al., 2015)

6.1.1.2 Status of Participation in DECOVALEX Task B2

Task B2 focuses on coupled THMC modeling of a recently initiated full-scale EBS experiment conducted by the Japan Atomic Energy Agency (JAEA) at the Horonobe URL in Japan (Section 3.1.2.3). As a first modeling step, participating teams were asked to simulate a simplified 1D benchmark test with exact properties and boundary conditions given by the JAEA. This step allowed teams to get familiar with the problem setup and to conduct an initial model comparison for a simpler test problem before simulating the complex full-scale EBS experiment. The benchmark is a one-dimensional representation of the heater, buffer, and rock extending from the center of the overpack (heat source) out to 25 m. As shown in Figure 6-9, this includes 0.41 m of overpack, 0.72 m of bentonite buffer, and 23.87 m of rock. Figures 6-10 and 6-11 show selected simulation results, demonstrating good agreement between the five modeling teams participating in Task B2. As discussed below, teams have now moved to the next modeling steps, which are to conduct initial “blind” model predictions for the full-scale Horonobe EBS experiment followed by a calibration analysis using the first few months of monitoring data. Results are reported in Rutqvist et al. (2013), Zheng et al. (2014), and Zheng et al. (2015).

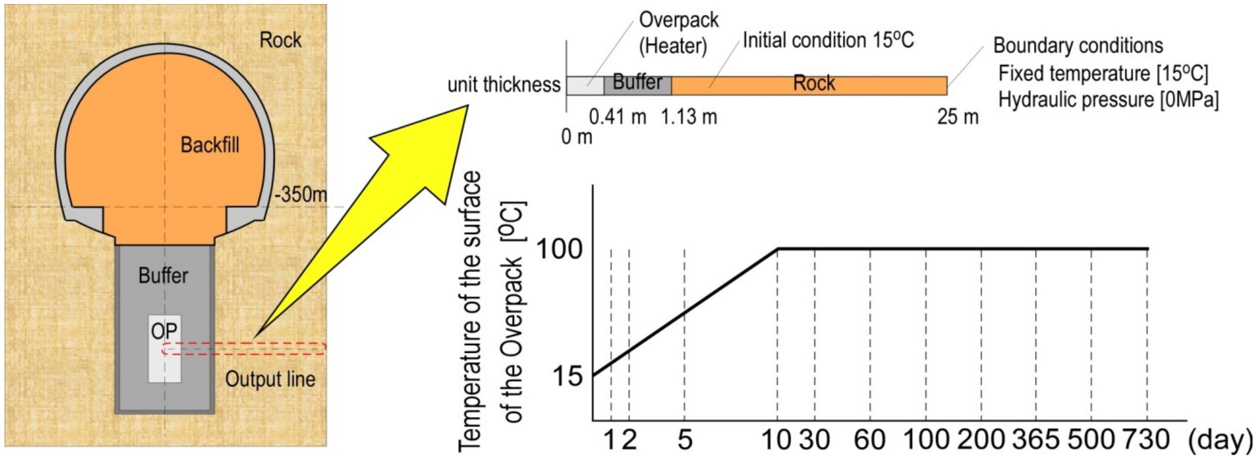


Figure 6-9. Definition of 1D benchmark test for Task B2 (from Rutqvist et al., 2013)

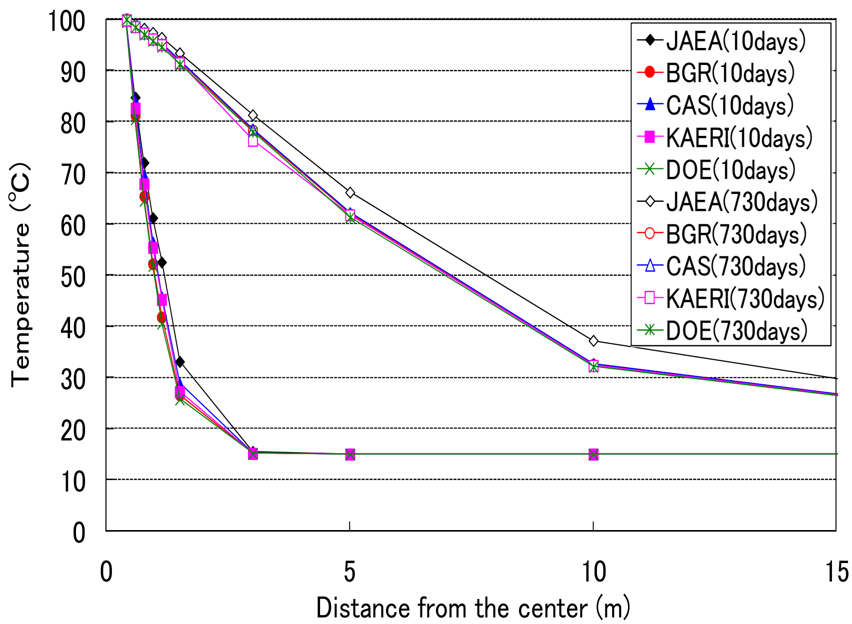


Figure 6-10. Task B2 Benchmark test: Comparison of simulated temperature as a function of distance from the center, for two time steps at 10 days and 730 days (from Zheng et al., 2014)

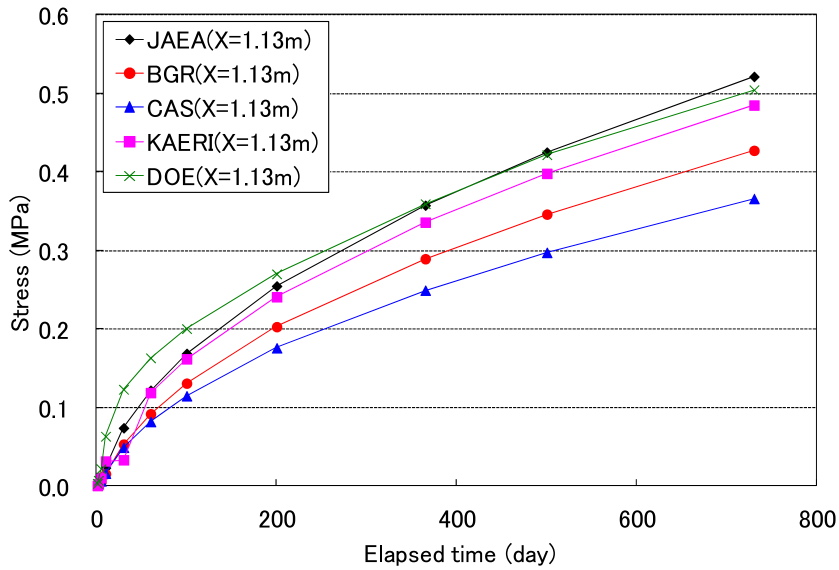


Figure 6-11. Task B2 Benchmark Test: Comparison of the simulated stress change at X=1.13m (from Zheng et al., 2014)

To conduct the predictive simulations for the Horonobe EBS experiment, the LBNL team developed a half symmetric 3D model, which includes half of the tunnel and half of the deposition hole (Figure 6-12), and explicitly represents all relevant materials, including mudstone rock, buffer, backfill, a sand layer at the rock/buffer interface, concrete lining, and plug. Preliminary simulations of the expected THM response were conducted for a heating period of about 2 years. Selected results of temperature evolution are shown in Figures 6-13 for points located in the buffer and near-field rock. When keeping the heater temperature constant at 100°C, the simulation shows that the temperature at the buffer-rock interface (P3, P4 in Figure 6-13) increases to about 60°C after 2 years.

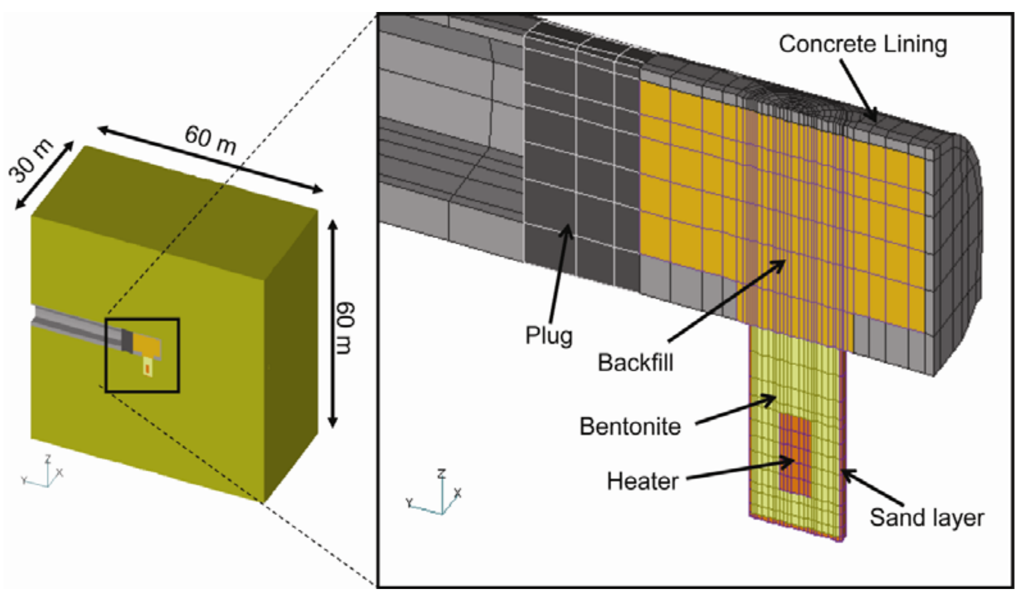


Figure 6-12. TOUGH-FLAC 3D numerical grid of the Horonobe EBS experiment (from Zheng et al., 2015)

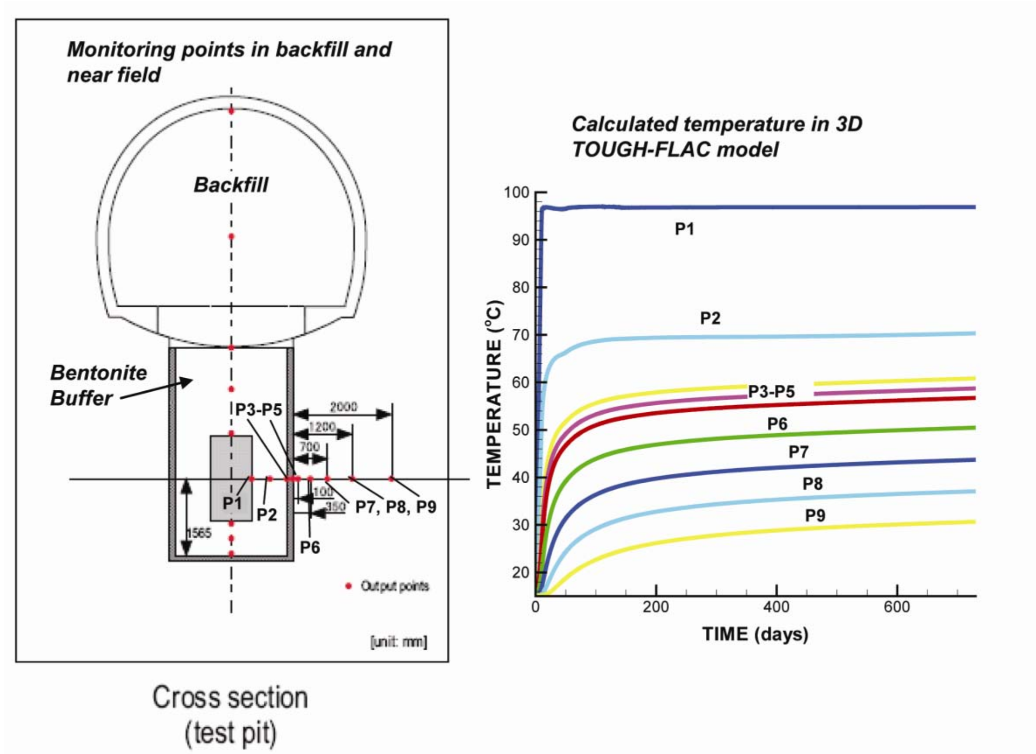


Figure 6-13. EBS Experiment: TOUGH-FLAC simulation results of temperature in the buffer and rock (from Zheng et al., 2015)

In addition to LBNL's prediction, four other international modeling teams are participating in Task B2, namely BGR from Germany, CAS from China, KAERI from Korea, and JAEA. The predictive results of the model predictions provided by all the DECOVALEX-2015 modeling teams have been compared. Figure 6-14 and 6-15 show examples of comparison of blind predictions, related to the evolution of temperature and liquid saturation in the bentonite buffer. The results are quite consistent and in good agreement between the modeling teams, though some outliers can be observed. The next step is to complete the calibration analysis using measured data to be provided by the JAEA.

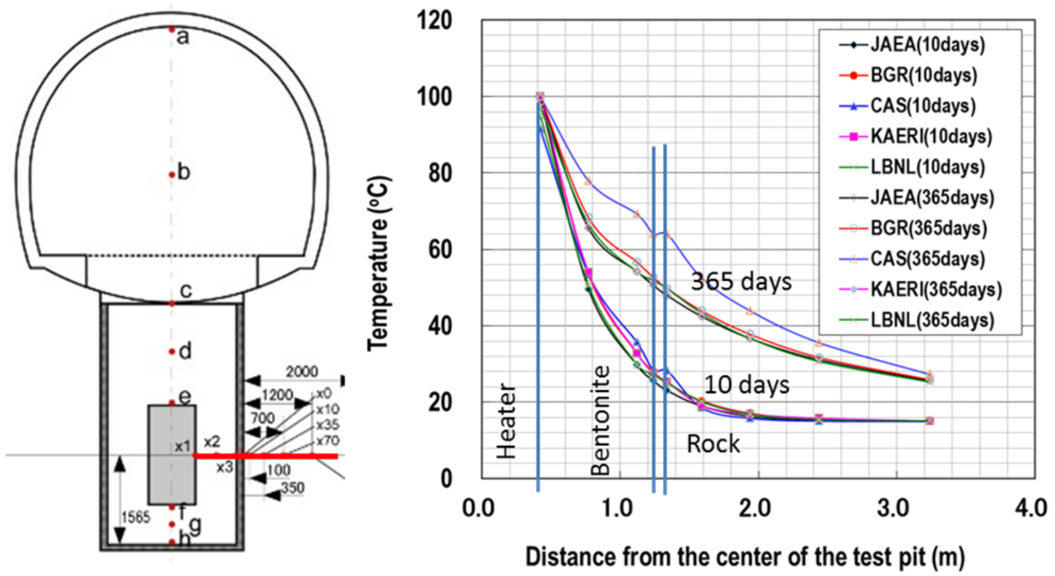


Figure 6-14. Comparison of simulated temperature profiles at 10 and 365 days among the DECOVALEX modeling teams (from Zheng et al., 2015)

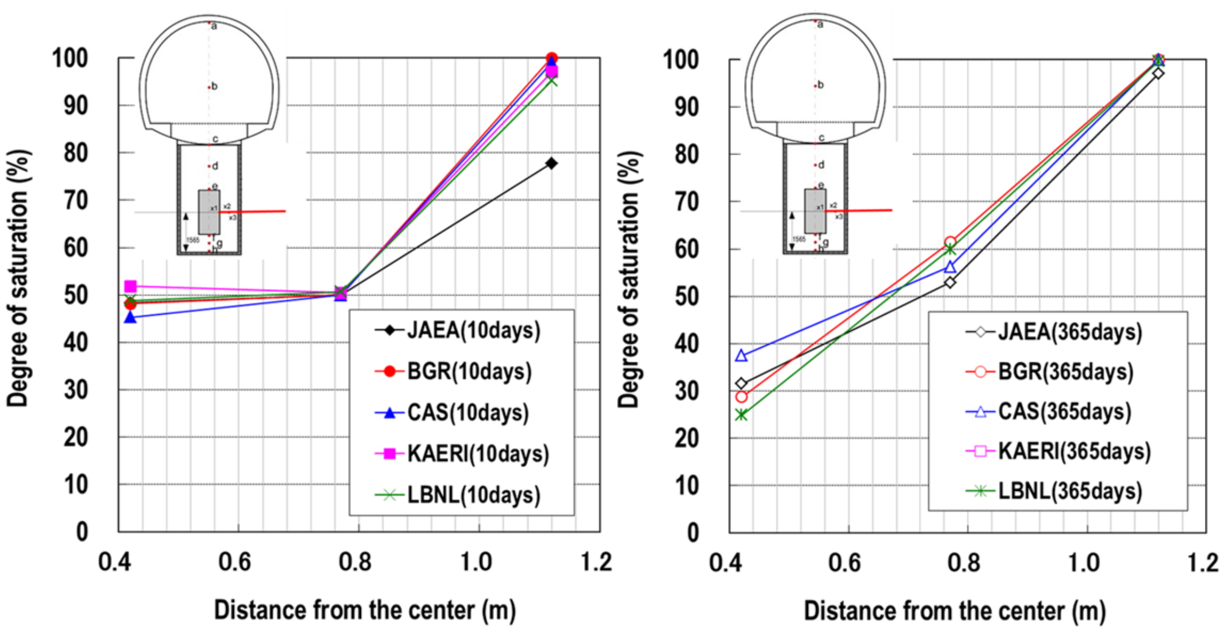


Figure 6-15. Comparison of simulated saturation profiles at 10 and 365 days obtained by the DECOVALEX modeling teams (from Zheng et al., 2015)

6.1.1.3 THM Modeling of FE Heater Test at Mont Terri

Enabled by DOE's formal partnership in the Mont Terri Project, LBNL is one of seven international modeling teams conducting THM simulations for the design of the FE Heater Test and for the evaluation of monitoring data. As mentioned in Section 3.2.2, this experiment has started its heating phase in February 2015 and is now the largest and longest-duration heater tests worldwide, with focus on both the EBS components and the host-rock behavior. Over more than a decade, the experiment will provide data useful for the validation of THM coupling effects regarding the processes in the host rock, while correctly accounting for (and examining) the conditions in the emplacement tunnel (temperature, saturation, and swelling pressure). Due to the 1:1 scale of the experiment, it is possible to achieve realistic temperature, saturation, and stress gradients in the emplacement tunnel and the host rock, which is extremely useful for THM model validation.

During the past three years, modeling teams have conducted design predictions for the FE Heater Test, developing conceptual models and selecting material properties from the review of available literature (papers and reports) on lab experiments and previous Mont Terri *in situ* tests. Several sets of scoping simulations were conducted to probe the relevance of coupled processes, evaluate their significance and parameter range, compare conceptual models, test sensitivity to input parameters, and summarize lessons learned before the onset of the experiment (parameter ranges, importance, expected response). This initial step was complemented with a restricted benchmark test for code comparison, in which properties and model geometry were defined by NAGRA. Modeling teams are now moving into a new modeling phase with evaluation, interpretation, and validation using measured data from the FE Heater Test.

In collaboration with NAGRA and other teams, LBNL has developed a sophisticated 3D TOUGH-FLAC model for the THM design predictions. This work is described in the FY14 milestone report entitled "*Investigation of Coupled Processes and Impact of High Temperature Limits in Argillite Rock,*" FCRD-UFD-2014-000493 (Zheng et al., 2014). The host rock is modeled with anisotropic properties considering bedding planes in the Opalinus Clay. An inclined TOUGH-FLAC mesh was created to accurately represent anisotropic thermal and hydrological behavior. Anisotropic mechanical material behavior is simulated using the FLAC3D ubiquitous joint model, with initial properties derived from excavation design analysis conducted by another FE Heater Test modeling team (Nater, 2012). In the ubiquitous joint model, weak planes are assumed along the bedding planes of the Opalinus Clay; in other words, the shear strength properties are different in the direction of bedding versus the direction across bedding. Bentonite behavior is accounted for with the Barcelona Basic Model (BBM). Figure 6-16 presents the 3D TOUGH-FLAC numerical grid of the FE experiment. This model grid includes all vital material components for the modeling of the FE experiment, including layered Opalinus Clay host rock, excavation-disturbed zone, tunnel, three heaters, bentonite buffer, concrete liner, and concrete plug. As in the real test, the predictive simulations start with an open tunnel at atmospheric pressure for one year, creating a pressure drop and hydraulic gradient around the tunnel. Thereafter, the model assumes instantaneous emplacement of the heater and buffer, and the heating period is simulated.

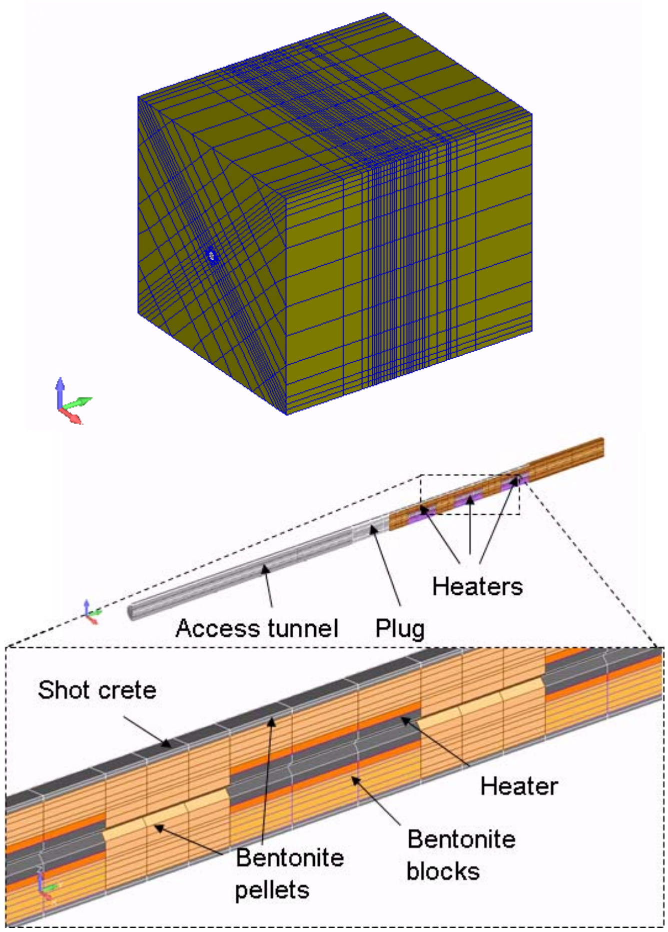
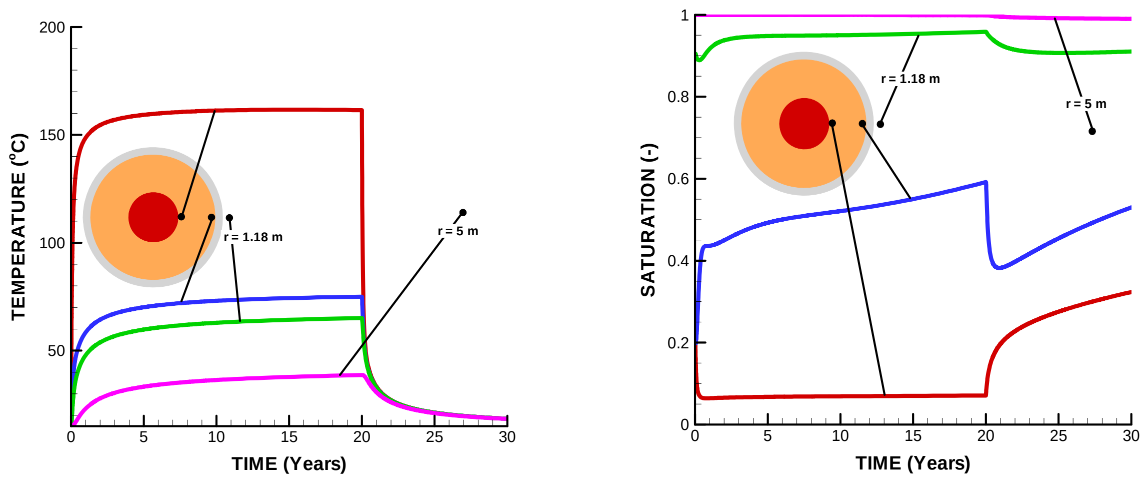


Figure 6-16. TOUGH-FLAC 3D numerical grid of the FE experiment (from Zheng et al., 2014)

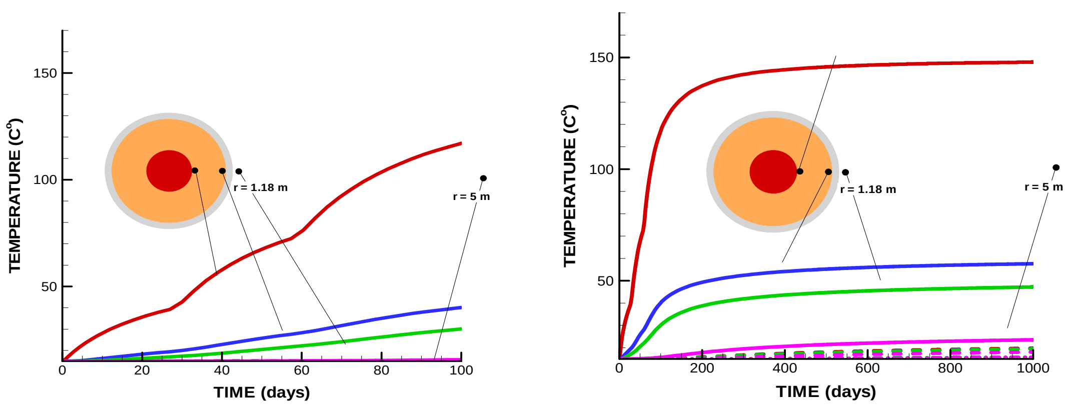
Figure 6-17 shows LBNL's initial prediction of temperature and saturation evolution, assuming the full 1500 W power in each heater operating over a 20-year period. In this case, the peak temperature at the buffer is as high as 160°C, i.e., considerably higher than the targeted 125°C to 135°C. In the experiment, the temperature should not exceed 150°C, because this could be damaging for some of the monitoring sensors. The high peak temperature at the canister surface is caused by the combined effects of low thermal conductivity of the buffer and the rock, as well as the high vapor diffusion coefficient that keeps the buffer dry around the heater. Modeling teams then explored alternative heating schemes, including staged heating, to better accommodate the targeted temperature constraints.

Figure 6-18 gives recent simulation results designing a staged heating schedule using only one of the three heaters, i.e., the one placed farthest into the tunnel, during the first few months of the experiment, The staged heating schedule was eventually adopted by the project leads to enable an early model calibration of the in situ thermal properties that can then be used to make a more reliable prediction of the peak temperature once the full thermal power is applied. This is done to ensure that the temperature will not be so high as to damage the monitoring system.



(a) (b)

Figure 6-17. Model prediction of (a) temperature and (b) liquid saturation for full power of 1500 W at each heater (from Zheng et al., 2014)



(a) (b)

Figure 6-18. Model prediction of temperature for staged power in first emplaced heater. The results in (a) and (b) are the same but using a different range on the time axis to highlight the early time behavior. Solid lines refer to evolution at the heater that is turned on, whereas dashed lines refer to evolution at heaters that are turned off (from Zheng et al., 2015).

6.1.1.4 Summary of Heater Test Modeling in Argillite Rocks

Over the past few years, UFD researchers have greatly benefited from participating in international activities for developing expertise and testing advanced models for coupled THM processes. As described below, LBNL scientists are now utilizing data and results from laboratory and field studies that have been and are being conducted with millions of R&D investments provided by international partners. UFD simulators are being verified and validated against these experimental studies, providing a robust modeling and experimental basis for the prediction of the complex long-term THM and THMC evolution of a multi-barrier waste repository system involving backfilled emplacement tunnels and argillite host formations. Specific FY2015 accomplishments of UFD scientists include:

- Validation of TOUGH-FLAC and characterization of THM properties was achieved through modeling of CIEMAT laboratory column experiments and interpretative simulation of the Mont Terri HE-E experiment.
- Benchmarking associated with the DECOVALEX-2015 Horonobe EBS Experiment demonstrated good agreement of UFD models with results of other international modeling teams, providing code-to-code verification of TOUGH-FLAC.
- Full-scale 3D models were developed for the Horonobe EBS Experiment and the Mont Terri FE Heater Test and initial model predictions of temperature and saturation evolutions were conducted for later comparison with measurements.
- Ongoing collaborative work in this area utilizes the full-scale 3D models of the *in situ* heater experiments—in particular the long-running Mont Terri FE experiment—for further comparison of simulation results with measurements and with the results of other international modeling teams.

6.1.2 UFD Participation in FEBEX-DP Experiment

6.1.2.1 Status of FEBEX-DP Activities

As described in Section 3.3.2, the FEBEX-DP project provides a unique opportunity to evaluating the long-term behavior of an engineered barrier that underwent continuous heating with natural resaturation for about 18 years. In FY15, LBNL scientists have been participating in the pre-dismantling modeling, with particular focus on the chemical alteration of the bentonite and how this alteration is affected by THM processes such as hydration, thermal osmosis, and swelling; this activity will continue in FY16 with post-dismantling modeling and interpretative analyses once dismantling results have become available. In FY16, UFD scientists from LBNL, LANL, and SNL will also participate in the sample analysis campaign of bentonite and its interfaces with other EBS components (i.e., metals, cement).

The ultimate goal of LBNL's modeling effort is to develop a coupled THMC model of the FEBEX-DP behavior tested against observation data. Specifically the following questions are to be answered with THMC modeling:

- What causes the hydration of bentonite to be slower than typically predicted by a Darcy flow model: Non-Darcian flow behavior, thermal osmosis that counteracts flow toward the heater, decrease of intrinsic permeability of the buffer due to changes in microstructure, or a combination of all these processes?
- What is the spatial density variation of the bentonite as a result of long-term hydration and swelling?
- What is the chemical evolution in the bentonite, especially the changes of more soluble minerals (gypsum, calcite and pyrite) and aqueous concentration, evolution of pH and Eh and alteration of smectite or other clay minerals?

As described in Zheng et al. (2015), LBNL's THMC simulations are conducted with TOUGHREACT-FLAC3D, which sequentially couples the multiphase fluid flow and reactive transport simulator, TOUGHREACT (Xu et al., 2011), with the finite-difference geomechanical code FLAC3D (Itasca, 2009). The coupling of TOUGHREACT and FLAC was initially developed in Zheng et al. (2012) to provide the necessary numerical framework for modeling fully coupled THMC processes. It was equipped with a linear elastic swelling model (Zheng et al., 2012; Rutqvist et al., 2013) to account for swelling as a result of changes in saturation and pore-water composition and the abundance of swelling clay (Liu et al., 2013; Zheng et al., 2014). A recent addition to the code is the capability of simulating Non-Darcian flow.

Model development for FEBEX-DP is being conducted in a sequence, starting with the development of a TH model, followed by development of separate THC and THM models, and eventually establishment of a fully coupled THMC model. In FY15, a preliminary THC model has been developed to provide scoping simulations of chemical changes and test the relevance of Non-Darcian flow behavior on the hydration of bentonite. THC model results were compared with TH data measured in the bentonite surrounding Heater 2, and with chemical data obtained from the 2002 dismantling of Heater 1 (chemical data for Heater 2 will become available in FY16). Example plots for temperature data and chloride concentrations in comparison with simulation results are given in Figures 6-19 and 6-20, respectively (Zheng et al., 2015).

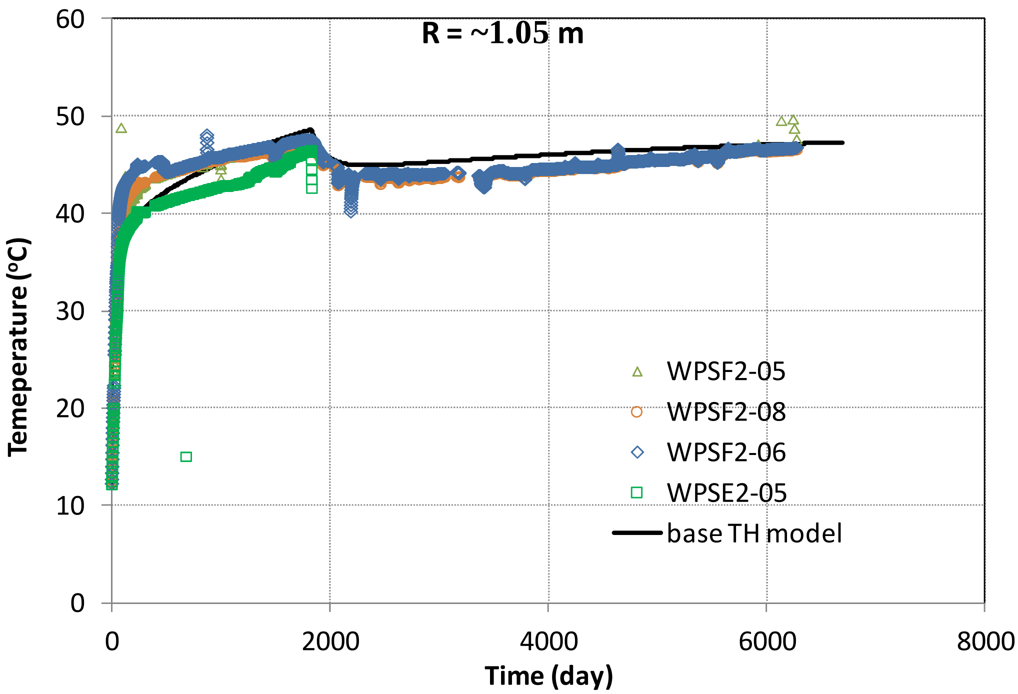


Figure 6-19. Temperature measured by sensors located at radial distance of 1.05 m in sections E2 and F2 of FEBEX Test and model results from the base TH model (from Zheng et al., 2015)

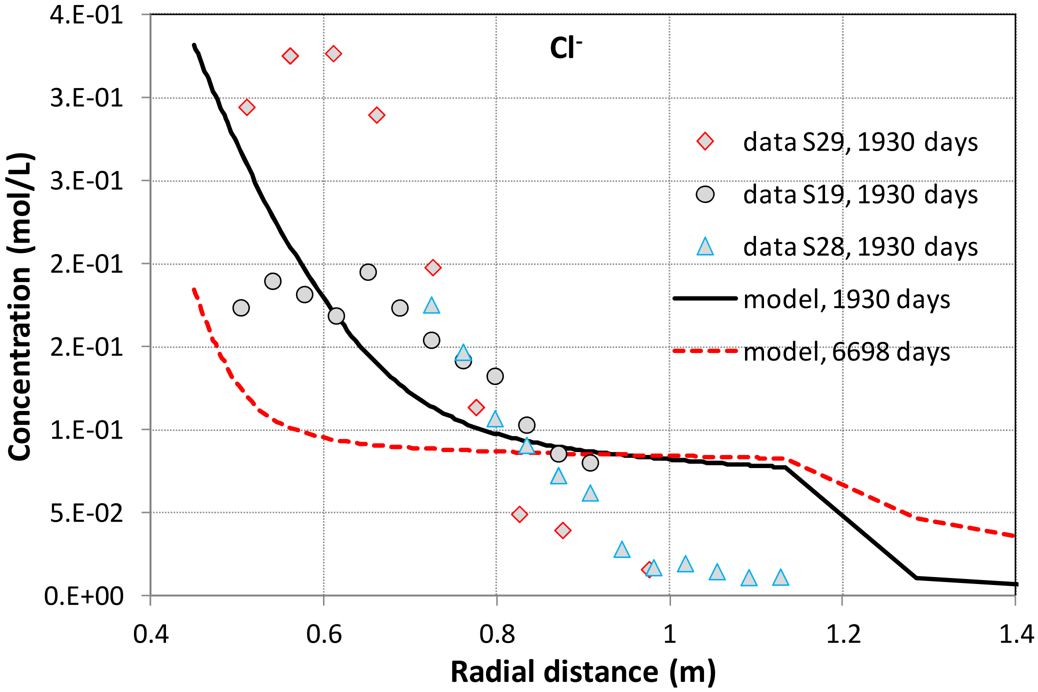


Figure 6-20. Concentration profile of chloride measured during dismantling of Heater 1 2002 (at 1930 days) and model results from the base model, for 1930 days and 6698 days (representative of Heater 2 dismantling in 2015) (from Zheng et al., 2015)

The key findings from this preliminary modeling work are as follows:

- For temperature, the match between measurements and simulation results is generally very good. Relative humidity behavior is more complex, and is not always well represented by the models. Adjusting key hydrological parameters such as permeability of bentonite and granite may lead to a better fit of measured relative humidity at given locations, but cannot explain relative humidity across the entire bentonite barrier. Hydromechanical processes (especially swelling) have to be considered in future work.
- Including Non-Darcian flow into the TH model leads to a significant underestimation of the relative humidity data in the entire bentonite barrier (even in bentonite near the bentonite/granite interface). The reason could be that the calibration of relative permeability curves for bentonite (and retention curves) already encompasses the nonlinear relationship between gradient and flux, which would obviate the consideration of Non-Darcian flow in the model. Non-Darcian flow under unsaturated conditions still needs more study.
- In comparison with the chemical data obtained after the dismantling of Heater 1 in 2002, the THC model captures the general trend of the concentration profiles of major cations and anions. However, the model overestimates the concentrations of most of these species in the bentonite near the bentonite/granite interface, which can be improved when mechanical change is included in the model, i.e., with THMC models.
- The preliminary predictions of the chemical changes between 2002 and the dismantling of Heater 2 in 2015 are that concentration levels will have continued to decrease in the bentonite near the heater; calcite will have dissolved and dolomite formed; and illite will have precipitated in the

bentonite near the bentonite/granite interface accompanied by the dissolution of smectite at the same place. In FY16, these preliminary predictions will be tested against dismantling analyses.

6.1.2.2 Future Plans for FEBEX-DP Activities

In FY16, the development of a THMC model for the FEBEX-DP test will continue. The following modeling tasks are planned:

- Mechanical processes will be added to the current THC model. Once the coupled THMC model is developed, mechanical-hydrological coupling relationships will be calibrated again measured stress, dry density, water content and relative humidity data.
- The chemical model will be further refined. Once the concentration profile for chloride can be matched by the THMC model, predictions will be made for other chemical species and mineral phases.
- Once the corrosion of the steel liner is analyzed, chemical changes of steel will be included in the chemical model to evaluate the interaction of steel and bentonite.

Ultimately, after the THMC models for FEBEX *in situ* test are fully validated with data, they will be used to explore long-term THMC changes under high-temperature conditions.

In FY16, UFD scientists will also participate in the sampling and analysis campaign of bentonite interfaces with other EBS components (i.e., metals, cement). LANL scientists will perform initial forensic analysis of selected samples (focusing on bentonite-metal, bentonite, and bentonite-cement segments) to understand the alterations that took place during the 18-year experiment. Following the forensic analyses, a series of hydrothermal experiments will be conducted to expand the thermal knowledge of this particular bentonite system and compare the results to ongoing LANL experiments conducted on other bentonite systems. Results from these hydrothermal experiments will elucidate bentonite alterations during long-term heating under controlled conditions beyond what was observed in the FEBEX project.

LBNL and SNL plan to collaborate on the study of micro-cracks in FEBEX-DP samples. Micro-cracks could have formed during heating and drying, but then might have healed during hydration. Such a study will not only facilitate better understanding of potential flow paths in bentonite, but will also shed light on the self-healing of excavation disturbed zone (EDZ) in the argillite host rocks, because of the similarity in the controlling processes. LBNL will use the synchrotron light source at LBNL to examine the micro-cracks at a resolution of ~750 nm. These microCT images will provide a dynamic of the evolving micro-cracks. In a second step, the microCT results will be used by SNL to select target locations for FIB/SEM analysis and serial sectioning to image micro-cracks at a smaller scale but higher resolution. Together, these tests will yield a multiscale characterization of micro-crack behavior.

6.1.3 DFN Modeling of the HG-A Experiment at Mont Terri

To more accurately characterize and model excavation-damage-zone evolution and its impact on flow and transport, LBNL has developed a new modeling approach for studying hydro-mechanical coupled processes, including fracture development, within geologic formations. This is accomplished through the novel linking of two codes: TOUGH for subsurface multiphase flow based on the finite volume method, and RBSN (Rigid-Body-Spring-Network) for discrete (lattice) representation of material elasticity and dynamic fracture development/propagation. The RBSN formulation is based on the concept of the Rigid-Body-Spring model, first introduced by Kawai (1978), in which the material constitution is represented as a collection of rigid bodies connected by spring sets. TOUGH is used to simulate relevant scalar quantities (e.g., temperature, pressure, and degree of saturation) associated with fluid flow and heat transport, whereas RBSN accounts for mechanical quantities (e.g., displacement, strain, and stress) of interest. The TOUGH-RBSN simulator predicts fracture evolution, as well as mass transport through fractured porous rock, under dynamically changing thermal-hydrologic and -mechanical conditions. The modeling approach is facilitated by a Voronoi-based discretization technique common to both codes, capable of representing discrete fracture networks embedded in a porous matrix. Further details on this method and UFD-related applications are provided in Section 3 of the *Report on Investigation of Coupled Processes and Impact of High Temperature Limits in Argillite Rock*, FCRD-UFD-2014-000493, August 2014 [Zheng et al., 2014]). More recent developments of the TOUGH-RBSN simulator, including a new dynamic simulation framework for RBSN that can be easily parallelized, are described in Zheng et al. (2015).

In FY13 and FY14, LBNL tested its new capabilities using data from the ongoing HG-A experiment at Mont Terri (Section 3.2.3). This experiment examines gas paths through the near-field host rock affected by the evolution of the damage zone. Several hydraulic and gas injection tests have been conducted, and a detailed discrete fracture mapping study was performed. The test is therefore a valuable testbed for discrete fracture and THM modeling capabilities. However, application to the HG-A experiment required a modification to the standard RBSN approach to account for anisotropic elastic properties of the RBSN spring sets. In the standard RBSN, the spring sets are oriented randomly as defined by the Voronoi element structure. In the new scheme, by comparison, all the spring sets are aligned with the principal bedding direction. The spring coefficients are defined in global fabric coordinates, where two orthogonal axes are normal and parallel to bedding, respectively. The anisotropic modeling scheme was validated through comparison with uniaxial compression tests for transversely isotropic rock specimens from Mont Terri. Cylindrical core samples were subjected to unconfined uniaxial compression, in which the loading direction formed an angle relative to the bedding plane. TOUGH-RBSN simulations were conducted for seven cases of fabric orientation relative to core sample axis with $\beta = 0^\circ, 15^\circ, 30^\circ, 45^\circ, 60^\circ, 75^\circ, 90^\circ$. Selected damage patterns are shown in Figure 6-21.

An initial set of TOUGH-RBSN simulations for the HG-A experiment focused on the excavation damage observed in the micro-tunnel (Figure 6-18). The partial damage and exfoliations observed along the tunnel have been mainly attributed to the anisotropic strength characteristics of the rock. The relative weakness of the rock orthogonal to the bedding and the weakness near faults intercepting the tunnel, as depicted in Figure 6-18, result in the nonuniform damage around the excavation wall. Simulated damage patterns are shown in Figure 6-19. Damage zones are more prominent at the tunneling wall tangential to the bedding planes, similarly to the failure characteristics seen in Figure 6-18. For identification of failure modes, individual fracture segments are drawn in different colors: blue and red segments represent tensile and shear failure modes, respectively. Tensile fracturing is concentrated at the borehole boundary, due to the lack of constraints against the pore pressure acting towards the center of the tunnel. This failure feature can be supported by observation of the deformation around the borehole. Figure 6-19c depicts the deformed shape of the tunnel, in which the deformation is exaggerated for better visibility. Voronoi cells adjacent to the borehole come off the body, which indicates tensile failure. For FY15, LBNL had planned to conduct a second set of HG-A simulations modeling the hydraulic and gas injection tests conducted at the site, in particular those that may have caused additional damage in the EDZ; however, these plans were abandoned because of budget constraints. Currently discussed is the possibility of using TOUGH-RBSN for damage modeling related to long-term gas generation from canister corrosion in low-permeable backfill, a possible modeling task in the next DECOVALEX Project phase (Section 3.1.3.1).

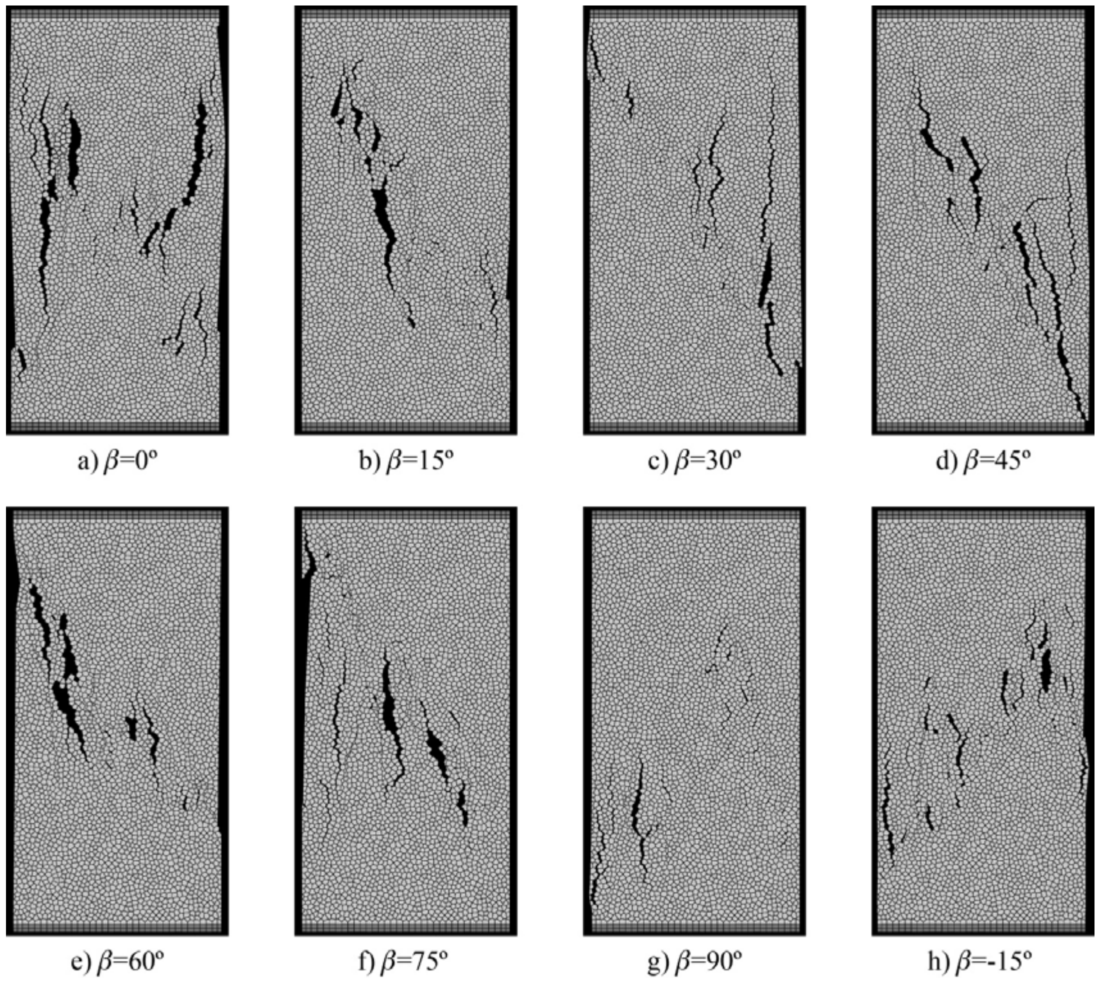


Figure 6-21. Fracture patterns of the specimens with various orientations of fabric forming the angle of ß with the loading axis. Note that the positive angle indicates counter-clockwise rotation from the vertical orientation (from Zheng et al., 2014)

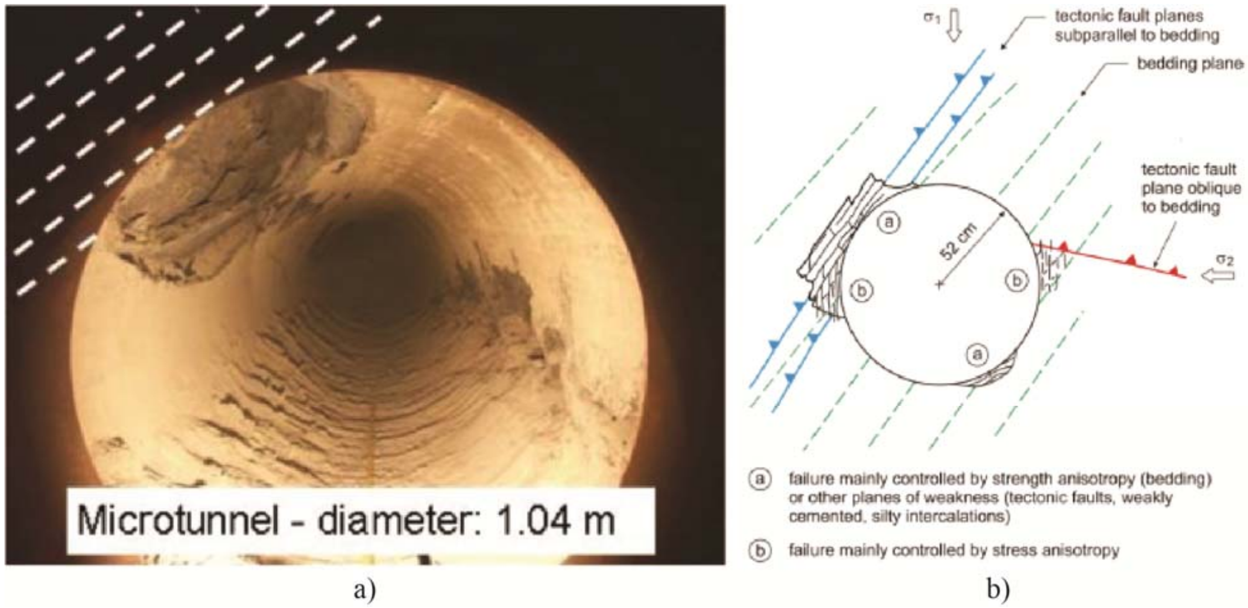


Figure 6-22. a) Excavation damage viewing from the HG-A Niche towards back end (from Marschall et al., 2006); and b) Conceptual diagram of the damage zone (from Lanyon et al., 2009)

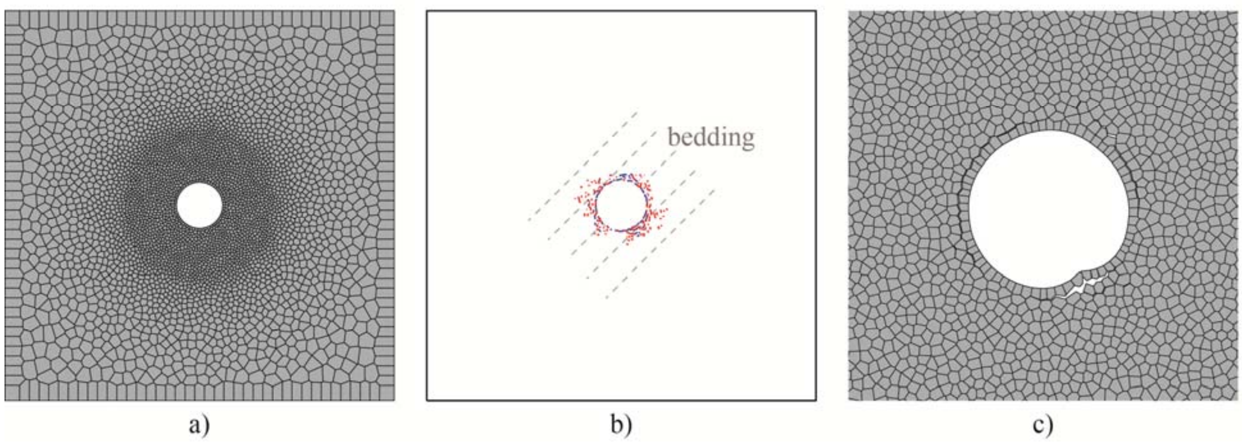


Figure 6-23. a) Discretization of the computational domain for the HG-A test simulation; b) nonuniform fracture pattern around the tunnel; and c) deformed shape of the borehole (from Zheng et al., 2014)

6.1.4 DFN Modeling of BRIE Experiment at Äspö Hard Rock Laboratory

Researchers at LANL have been developing novel discrete fracture network (DFN) approaches for modeling flow and transport in the near- and far-field domains of sparsely fractured crystalline formations (e.g., Section 2 in Milestone Report "*Crystalline and Crystalline International Disposal Activities,*" FCRD-UFD-2014-000495 [Dittrich et al., 2014], and Section 1 in Milestone Report "*Crystalline and Crystalline International Disposal Activities,*" FCRD-UFD-2015-000602 [Viswanathan et al., 2015]). In FY14, LANL started applying these capabilities (referred to as DFNWORKS) to the ongoing BRIE Experiment at Äspö Hard Rock Laboratory (see Section 3.4.2.1), where the water-bearing fractures have been mapped and their interaction with the bentonite backfill in a vertical deposition hole is being measured (Section 3.4.2). The main objectives of the work are to test and refine the DFN modeling capability using the BRIE site as a well-characterized demonstration site. While the development of DFN capabilities continued in FY15, there was no additional work on BRIE conducted this fiscal year. Therefore, we briefly summarize below the FY14 activities at LANL, and point out that there are plans for continued development of the DFN computational suite, including further application of the suite to model/interpret data sets related to SKB GWFTS Task Force activities, such as the proposed Task 9 (LTDE-SD at the Äspö HRL in Sweden, REPRO project at Onkalo in Finland) (see Section 3.4.2.2).

The scope of the BRIE modeling task is to simulate wetting of the bentonite in the emplacement boreholes (see Section 3.4.2.1). This requires that flow in the fracture network near the boreholes also be modeled. The DFN grids are locally two-dimensional whereas the emplaced bentonite requires a conventional three-dimensional space-filling grid. As a preliminary step in the BRIE modeling, LANL's DFN modeling capability needed to be extended to allow for hybrid DFN/volume grids. The procedure used to create hybrid DFN/volume meshes is illustrated for a simple example in Figure 6-24. In this example, the interior of a cylinder is to be meshed and merged with a DFN grid in the nearby rock volume. A DFN is first generated using the procedures described previously (Painter et al., 2012; Hyman et al., 2014). The generated DFN ignores the volume to be meshed. However, before the DFN is meshed, interfaces between fractures and the cylinder to be meshed are identified. A two-dimensional mesh is then created on each fracture in a way that conforms to the fracture intersections and to the fracture-volume interfaces (Figure 6-24A). In the second step, nodes on the fractures within the volume to be meshed are removed (Figure 6-24B). A tetrahedral mesh that conforms to the fracture intersection is then created within the cylinder. In the final step, the tetrahedral mesh and the DFN mesh are merged and duplicate nodes removed (Figure 6-24C). The LaGriT software (Los Alamos Grid Toolbox, 2011) was used to execute the meshing calculations.

Using the hybrid procedure explained above, the LANL team developed a BRIE model for a 40 m × 40 m × 40 m cube to simulate flow in the fractured granite surrounding two BRIE boreholes as well as flow in the bentonite-filled boreholes themselves. One typical meshed realization of the BRIE DFN with three deterministic fractures and two BRIE boreholes is shown in Figure 6-25. For this preliminary simulation, the lower cutoff for fracture length was increased to 1.0 m to reduce the size of the network, with appropriate adjustments to the fracture density. The network contains approximately 3500 stochastically generated fractures. Initial results for rewetting of the BRIE experiment boreholes for two realizations of the DFN are shown in Figure 6-26 at 3 months, 6 months, and 12 months. Little difference is noted between the two realizations. 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. This dependence of saturation on distance from the fracture intersection is attributed to the shape of the capillary pressure versus saturation curve, which provides for strong suction at lower saturation values (Section 3 in Dittrich et al., 2014). The two realizations of the DFN with boreholes in place is an important demonstration of an advanced modeling capability combining volume and DFN meshes, and incorporating complex geometries.

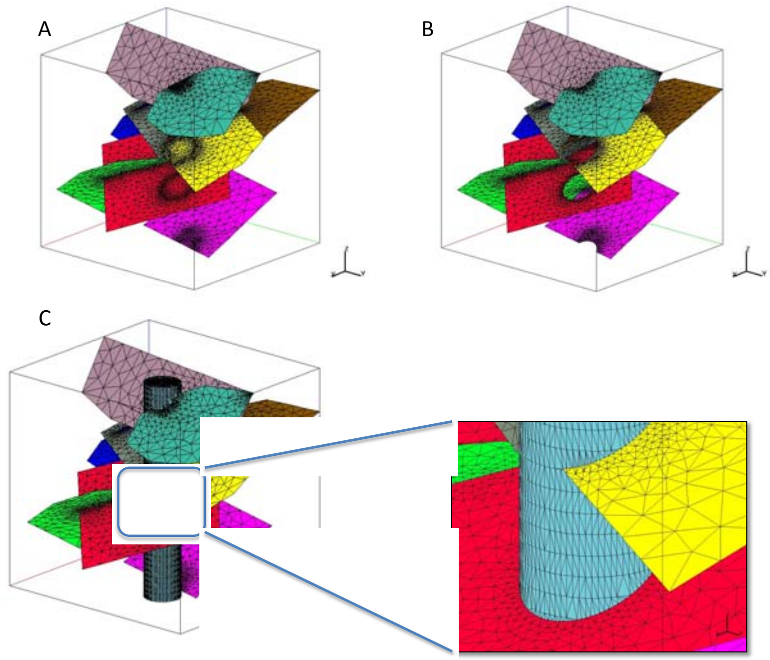


Figure 6-24. Example showing the creation of a hybrid tetrahedral/DFN mesh. Such hybrid meshes were required to model the rewetting of bentonite in the BRIE (from Dittrich et al., 2014).

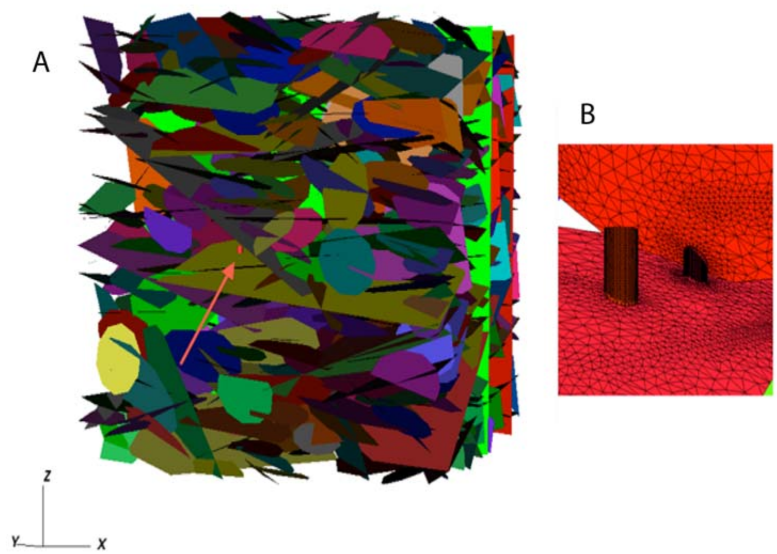


Figure 6-25. Computational mesh for the three-dimensional model of the BRIE experiment. The DFN and boreholes are shown in A. The arrow indicates the position of one of the boreholes. A detail from the computational mesh showing the merged DFN and tetrahedral mesh is shown in B (from Dittrich et al., 2014).

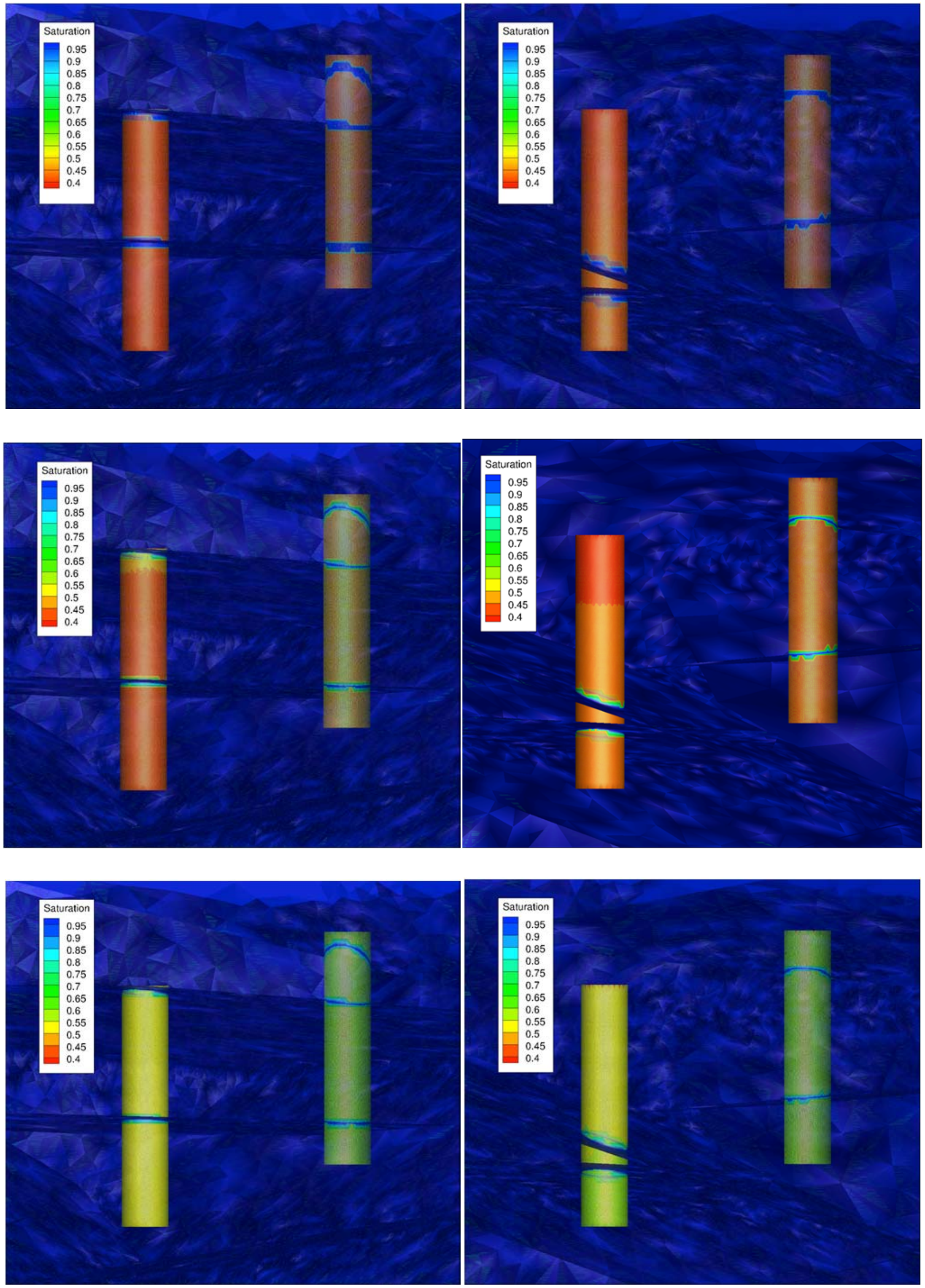


Figure 6-26. Details from two simulations of rewetting of the BRIE experiment boreholes. Results from one realization of the DFN are shown in each of the two columns. The top row is at 3 months, the middle row is at 6 months, and the bottom row is after one year of rewetting (from Dittrich et al., 2014).

6.1.5 Thermal-Hydrologic-Mechanical-Chemical (THMC) Processes in Single Fractures

Since 2014, SNL scientists have participated as DOE's modeling team in the interpretation and modeling of DECOVALEX Task C1, which uses data from single-fracture-flow laboratory experiments to model complex coupled THMC processes, in particular looking at the linkage of thermal stresses mediating chemical effects, and conversely of chemical potentials mediating mechanical behavior (e.g., pressure solution) (see Section 3.1.2.5). A mechanistic understanding of THMC-induced fracture opening and closure in geologic media is of significant importance to radioactive waste isolation (e.g., radioactive waste disposal and carbon sequestration and storage). It has been observed that, under certain circumstances, a fracture can undergo either opening or closure or switch from one regime to another. Fracture evolution involves a complex set of coupled physical and chemical processes, including stress-mediated mineral dissolution and precipitation, fluid flow and transport, mechanical deformation, etc. In FY15, SNL researchers formulated a dynamic model for subsurface fracture opening and closure (Wang et al., 2015). It is assumed that a fracture plane can be represented with isolated contacting asperities and connected aperture channels that run through between the asperities. It is further assumed that the cross-section of an individual aperture channel can be described as a truncated ellipse defined by the intersection of two identical ellipses. The model explicitly accounts for the stress concentration around individual aperture channels and the stress-activated mineral dissolution and precipitation. A preliminary model analysis demonstrated the importance of the stress-activated dissolution mechanism in the evolution of fracture aperture in a stressed geologic medium. The model provides a reasonable explanation for some key features of fracture opening and closure observed in laboratory experiments, including a spontaneous switch from a net permeability reduction to a net permeability increase with no changes in experimental conditions (Figure 6-27).

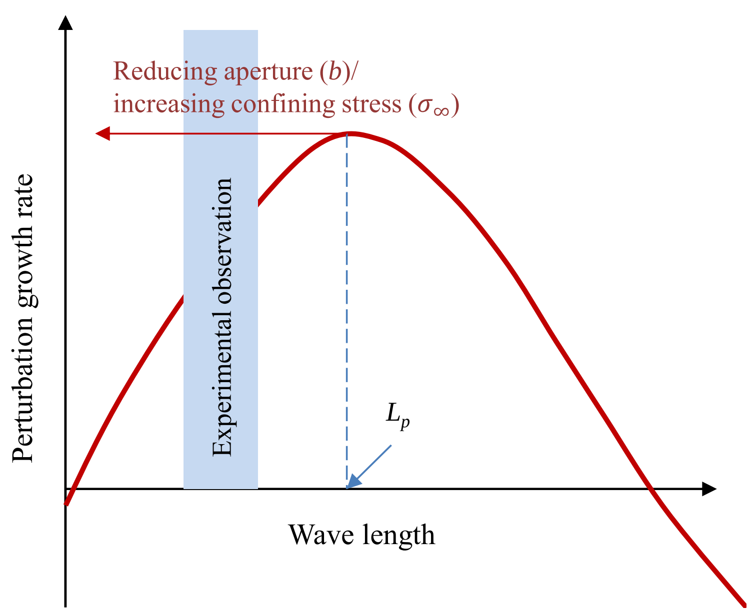


Figure 6-27. Spontaneous initiation of aperture channeling. As the fracture aperture reduces due to pressure dissolution, the preferred wave length of dissolution fingering decreases. Once the preferred wave length falls within the experimental observation range, a spontaneous initiation of preferential channeling can be observed. This may be responsible for the observed spontaneous switch from a net permeability reduction to a net permeability increase with no changes in a limestone fracture experiment (from Wang et al., 2015).

6.1.6 Salt Geomechanics Modeling and Benchmarking

A joint benchmarking study on HM and TM processes in salt between German groups and SNL has been officially extended to include two additional benchmarking problems based on *in situ* full-scale tests conducted in the early 1980s at WIPP. Modeling exercises compare an isothermal mining development test (WIPP Room D) to a heated "overtest" for simulated defense high-level waste (WIPP Room B). Calculations are isothermal, thermal-mechanical uncoupled, and thermal-mechanical coupled. Sandia uses a state-of-the-art Sandia Integrated Environment for Robust Research Algorithms (SIERRA) solid and thermal mechanics computer codes (Argüello, 2014), while the German partners use their respective codes and models as described by Hampel et al. (2012; 2013). All calculations use highly advanced constitutive laws that mathematically describe deformational processes inherent to those found in nuclear waste repository environment. The first goal of the project is to check the ability of numerical modeling tools to correctly describe relevant deformation phenomena in rock salt under various influences. International collaboration on model benchmarking is complemented immensely by additional testing of WIPP salt cores by German research laboratories. In concert with benchmarking of WIPP in situ experiments, German research groups are parameterizing their respective model variables through a series of special laboratory tests on WIPP salt. Thus their codes and models, which have been thoroughly calibrated against in situ experiments conducted in domal salt formations, will be appropriately parameterized for generic salt repository analysis with the inclusion of parameters representative of bedded salt (Hansen et al., 2015).

In a parallel US-German effort, researchers from LBNL have been collaborating with a research group led by Professor Lux in Germany at the Clausthal University of Technology (TUC) on modeling coupled THM processes in salt. LBNL incorporated into the TOUGH-FLAC simulator an advanced geomechanical constitutive model for rock salt developed by the TUC group (the Lux/Wolters model), a model that can handle creep, damage, sealing, and healing of the salt as a function of stress, temperature, and pore pressure. In FY15, using the TOUGH-FLAC simulator, LBNL and TUC have started working on THM benchmarking studies involving the TSDE (Thermal Simulation for Drift Emplacement) test conducted in the Asse Mine in the 1990s, Germany (see Section 4.2). A 3D (86,000 elements) TOUGH-FLAC model was developed and applied to simulate the TDSE behavior and compare simulation results with the observations (Figures 6-28 and 6-29). This is the first time this experiment has been modeled in a complete THM analysis (all previous analyses of TSDE have been limited thermal-mechanical processes, ignoring multiphase flow hydraulic processes). The modeling of the TSDE also provides the opportunity to calibrate stationary creep parameters at very low deviatoric stress and extremely slow loading that are not available from current laboratory tests. Good agreement was achieved between modeled and experimental data, involving drift closure and compaction of the EBS (crushed salt), thus providing validation of both host rock and crushed salt constitutive models and their implementation into the TOUGH-FLAC simulator. More details are provided in Milestone Report "*Modeling Coupled THMC Processes and Brine Migration in Salt at High Temperatures*," FCRD-UFD-2014-000341 (Rutqvist et al., 2015).

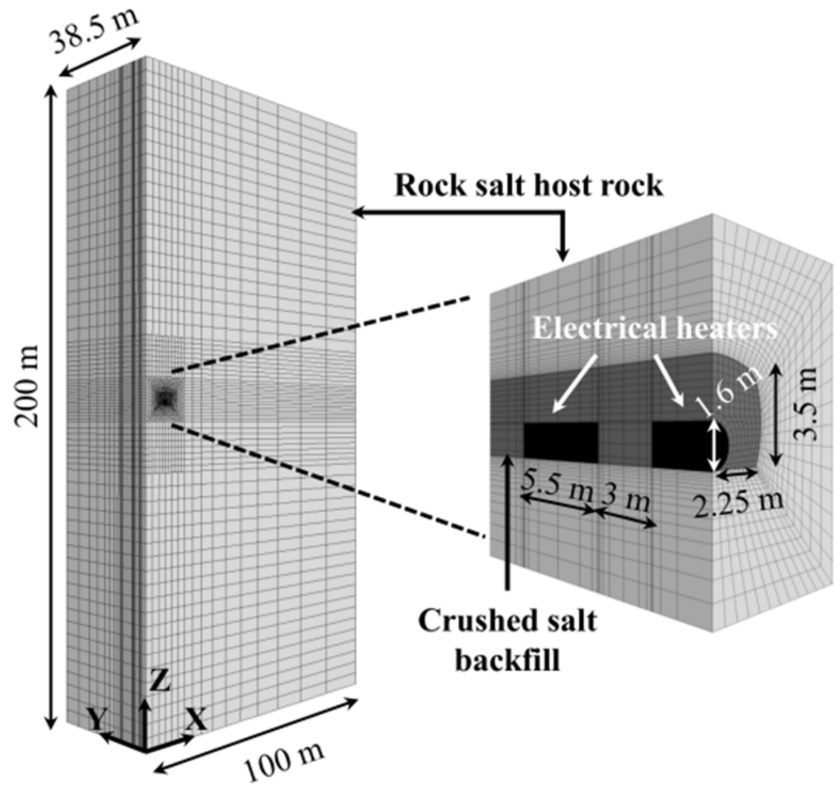


Figure 6-28. TSDE test: views of the initial mesh used in the geomechanics sub-problem. The main dimensions of the model are also shown (from Rutqvist et al., 2015).

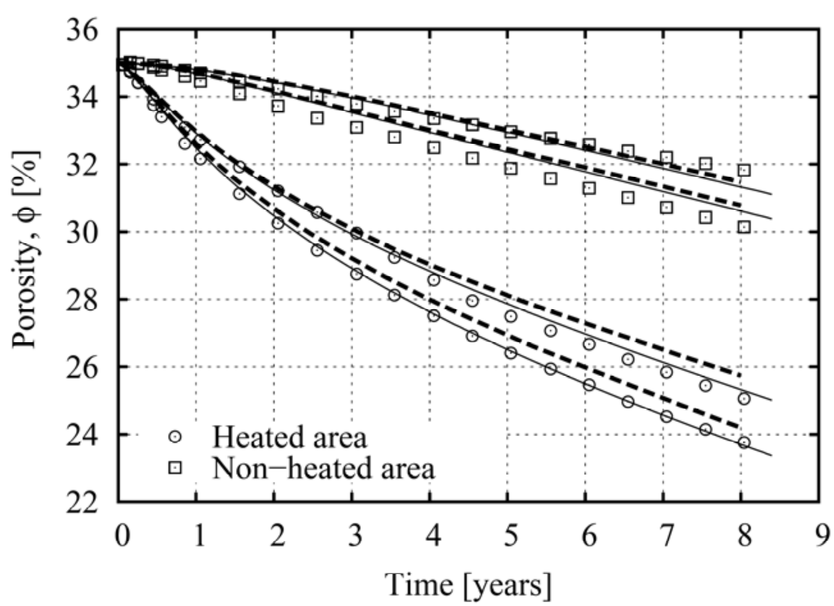


Figure 6-29. TSDE test: backfill porosity in the heated area and in the non-heated area. Points represent measurements, solid lines correspond to TOUGH-FLAC and dashed lines correspond to FLAC-TOUGH (from Rutqvist et al., 2015).

6.2 Fluid Flow and Radionuclide Transport

6.2.1 Using Environmental Tracers to Estimate Fracture-Network Properties: Application to the Bedrichov Tunnel Experiment

SNL scientists have also participated as DOE's modeling team in the interpretation and modeling of DECOVALEX Task C2, which is the Bedrichov Tunnel Experiment in the Czech Republic (see Section 3.1.2.5). The task utilizes a dataset of environmental tracers and discharge in the Bedrichov Tunnel. The expectation is that environmental tracers can provide valuable information for constraining parameters controlling flow and transport and making better predictions of contaminant transport in fracture network systems. The high-resolution groundwater discharge data measured in the Bedrichov Tunnel—along with measurements of stable isotopes of water, tritium, tritiogenic ^{3}He and other noble gases, as well as dissolved chlorofluorocarbons—provide a unique data set against which to test and calibrate numerical models of groundwater flow and solute transport in fractured media. The goal of Task C2 is to model groundwater flow and transport of environmental tracers in the fracture systems surrounding the Bedrichov Tunnel and utilize this data to constrain fracture-network parameters.

In previous work, consistent with the modeling steps defined for Task C2, SNL scientists initially developed a lumped parameter model for stable isotope, tritium and CFC-12 transport at the Bedrichov Tunnel site and compared model results to measured data (Wang et al., 2014). The lumped parameter model consistently predicts heavier isotopic values observed at the site, indicating preferential recharge of winter precipitation (Figure 6-30). PFLOTRAN, a multiphase, multicomponent reactive flow and transport simulator, was then used to simulate multiple environmental tracer concentrations in heterogeneous 2D and 3D domains (Figure 6-31). Fracture-zone permeability was calculated by matching the steady tunnel discharge to the appropriate values given in the description of Task C2. The modeling results demonstrate the usefulness of both the lumped parameter model and the PFLOTRAN code for evaluating flow and transport behavior in fractured crystalline rocks.

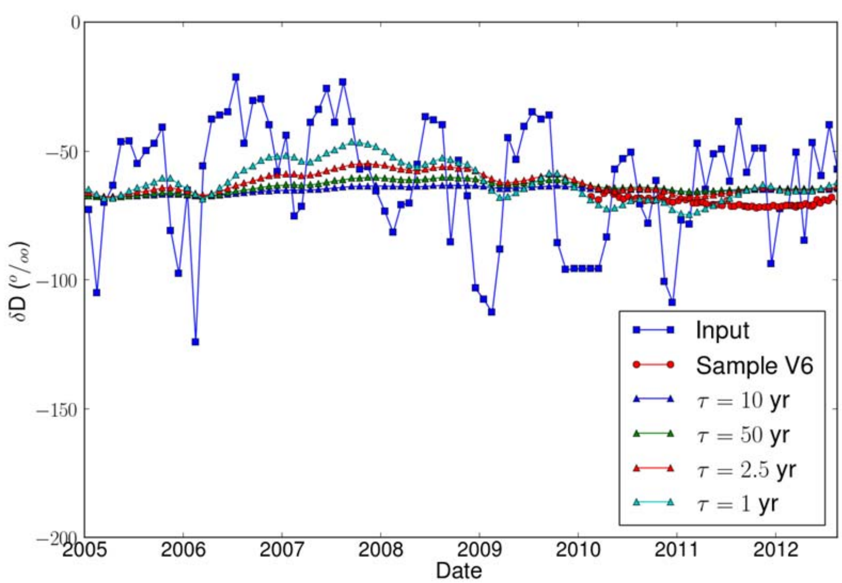


Figure 6-30. Measured and modeled stable isotope composition for the Bedrichov collection canal using the exponential age distribution (from Wang et al., 2014)

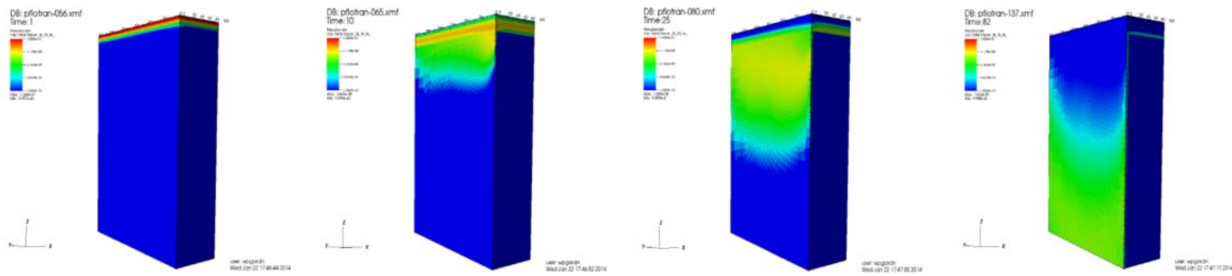


Figure 6-31. Transport sequence of tracer migration from a selected PFLOTRAN simulation run. Note that tracer concentration is contoured in log scale. Fracture plane on left side of domain, tunnel on right (front) of domain (from Wang et al., 2014) **.**

In FY15, SNL continued its interpretative modeling work for the Bedrichov site, utilizing several different conceptual models for isotopic transport at the site, including models that allow for a vertical fracture zone in addition to a background matrix permeability (Wang et al., 2015). In the latest set of simulations, the constant recharge used earlier models was changed to a transient recharge set as 20% of monthly average observed precipitation at the site. The steady state hydraulic field was used as the initial condition, and then the transient recharge was applied across the top of the domain. A transient defined concentration taken as monthly average isotopic concentration was then applied across the recharge zone. The estimated recharge, the calculated discharge, and the observed discharge are plotted below in Figure 6-32. Overall there is a reasonable order of magnitude match to the observed discharge. An annual transport sequence of $\delta^{18}O$, which highlights the seasonal changes in isotopic composition and its transport through the system, is shown in Figure 6-33.

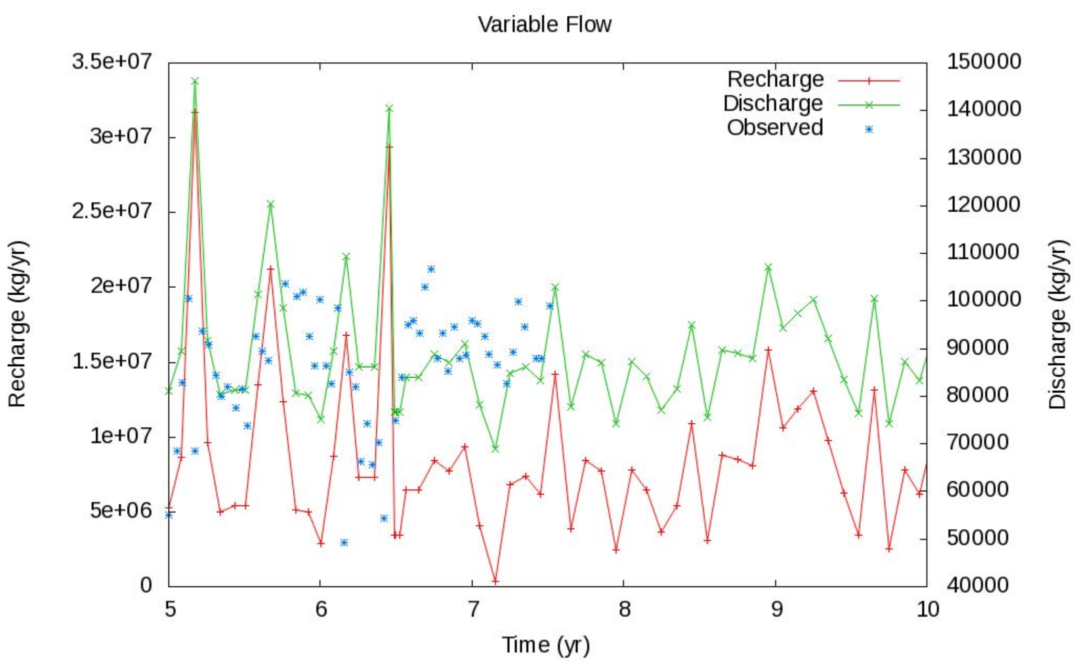


Figure 6-32. Transient recharge, modeled fracture discharge and observed discharge (Wang et al., 2015)

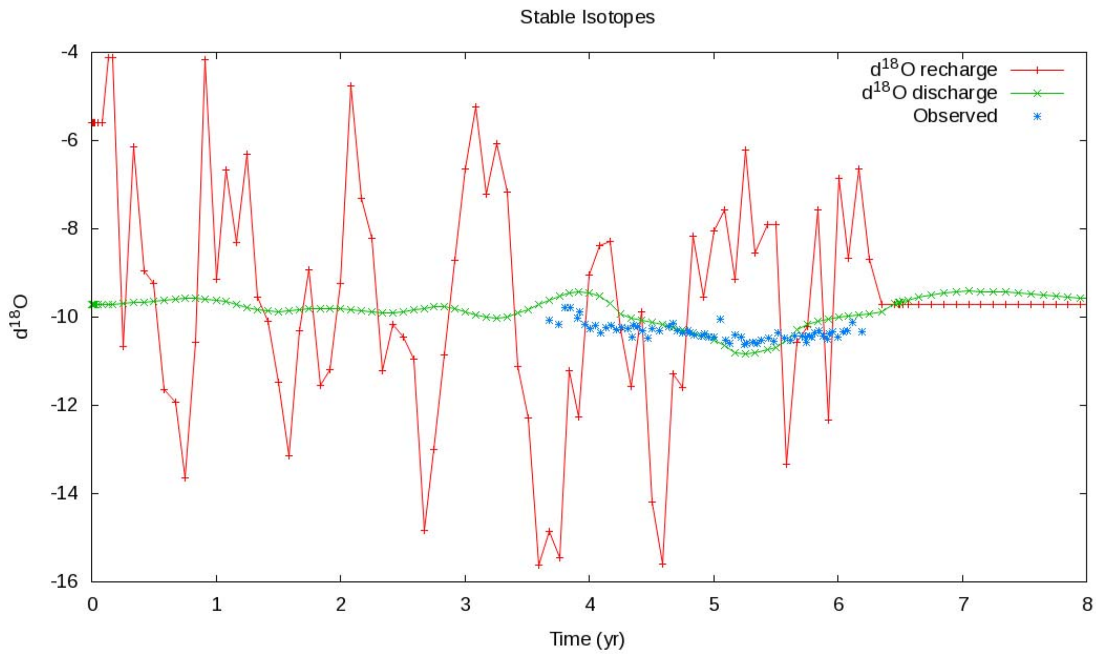


Figure 6-33. Transient $\delta^{18}O$ in precipitation (red line), modeled $\delta^{18}O$ in the fracture outflow (green lime) and observed $\delta^{18}O$ (blue dots) in fracture outflow (from Wang et al., 2015)

In FY15, the different modeling teams participating in DECOVALEX Task C2 conducted a thorough evaluation and comparison of their respective simulation models. For the most part the teams were able to match each other results, and overall all models reproduced the gross characteristics of hydraulic and tracer transport observed in the field. Understanding the discrepancies between models has proved to be a great learning experience for all teams and improved the understanding of the underlying mechanics of each code, and each codes strengths and limitations (Wang et al., 2015).

6.2.2 Diffusion-Reaction Modeling of the DR-A Experiment at Mont Terri

UFD researchers have also utilized international collaboration to test modeling approaches for radionuclide diffusion processes in compacted clay-based materials. In such materials (e.g., clay-rich rocks or compacted bentonite), the negatively charged clay particles are balanced by a cation-enriched electrical double layer (EDL). Radionuclide diffusion is affected by these electrochemical effects. While anions are likely to be excluded from this layer at high degrees of compaction, their concentration is decreased in the double layer even at lower degrees of compaction, and the tortuosity of the compacted clay with respect to chloride changes as well. Both of these contribute to slower diffusive transport rates of ions through compacted clay-rich materials (Bourg et al., 2003; Bourg et al., 2006; Leroy et al., 2006; Gonçalvès et al., 2007), an effect that becomes increasingly important as the compaction increases. For realistic performance predictions of radionuclide transport in the EBS and near-field rock, it is important to develop rigorous and yet practically useful approaches to modeling such diffusive processes.

LBNL has been pursuing two separate but related approaches to modeling ion diffusion through compacted clays. The first makes use of a Donnan equilibrium approach, in which a mean electrostatic potential is defined for the electrical double layer that balances the fixed negative charge of the clays. The volume of the EDL required for mass-balanced-based transport calculations is the product of the surface area of the clays and the width of the EDL, normally calculated as some multiple of the Debye length. The second approach involves the use of the Nernst-Planck and Poisson-Boltzmann equation (termed the Poisson-Nernst-Planck or PNP equation), which resolves the electrical potential as a function of distance from the charged clay surfaces. Both approaches predict that the electrical potential in the space between two clay layers does not decay to zero when the clay layers or interlamellae are closely spaced, and thus the water within the space does not have the same properties as "bulk water." A recent improvement of both methods now allows dynamic calculation of the width and the composition of the electrical double layer (or micro) porosity as a function of ionic strength (and other geochemical properties). Further details on this method and applications are provided in Section 6 of the Milestone Report "*Investigation of Coupled Processes and Impact of High Temperature Limits in Argillite Rock*," FCRD-UFD-2014-000493 (Zheng et al., 2014).

In FY13 and FY14, LBNL has been one of the international research teams involved in the DR-A Diffusion, Retention and Perturbation Experiment of the Mont Terri Project. As mentioned in Section 3.2.4, one of the geochemical perturbations investigated in this experiment was a dynamic change in ionic strength, which provides an extremely valuable set of validation data to test LBNL's new diffusive transport modeling capabilities with dynamic calculation of the EDL. We recall that the DR-A test consisted of a single borehole drilled in the Opalinus Clay that contained an ionic strength cocktail and anions, cations, and nonreactive tracers like tritium (HTO), operated in two stages: In the first stage through Day 189, the borehole cocktail was a 0.384 M ionic strength solution dominated by sodium. At Day 189, a higher ionic strength solution (1.135M) was circulated in the borehole without diluting the tracers (HTO, iodine, and bromine) in the cocktail. The higher ionic strength solution was allowed to diffuse out of the borehole through Day 412.

The diffusion simulations for the DR-A test conducted by LBNL assume a fixed total porosity for the Opalinus Clay, but with dynamic partitioning between the "bulk" and "EDL" porosities governed by the Debye length (which in turn is determined by the ionic strength, and thus variable over the course of the 412 day experiment). Selected results from the simulations, including the increase in ionic strength in the borehole-reservoir system at Day 189, are shown in Figure 6-34 in comparison to the measured data. One expects that the increase in ionic strength will lead to a decrease in the thickness of the EDL, and thus an increase in bulk versus EDL porosity. An increase in bulk porosity, in turn, is expected to allow for more effective diffusion of anions, and thus an increase in rate of loss from the borehole. Indeed, the anion (iodide and bromide) concentrations in the borehole show an increase in the rate of loss from the borehole starting about Day 189, the time when the ionic strength was increased. The simulation results also show an increase in the rate of loss from the borehole (solid blue for iodide), albeit slightly less pronounced, which is likely the result of the use of the same diffusion coefficients for the iodide and bromide in the EDL and bulk porosity. One expects that diffusion rates of anions in the EDL are smaller because of the greater tortuosity for the negatively ions versus the bulk fluid. The comparison between simulations and test results provides evidence that the electric double layer influences anion diffusion rates in the Opalinus Clay, that these rates are also affected by ionic strength, and that the new modeling approaches developed by LBNL can account for all relevant influences and effects on ion diffusion.

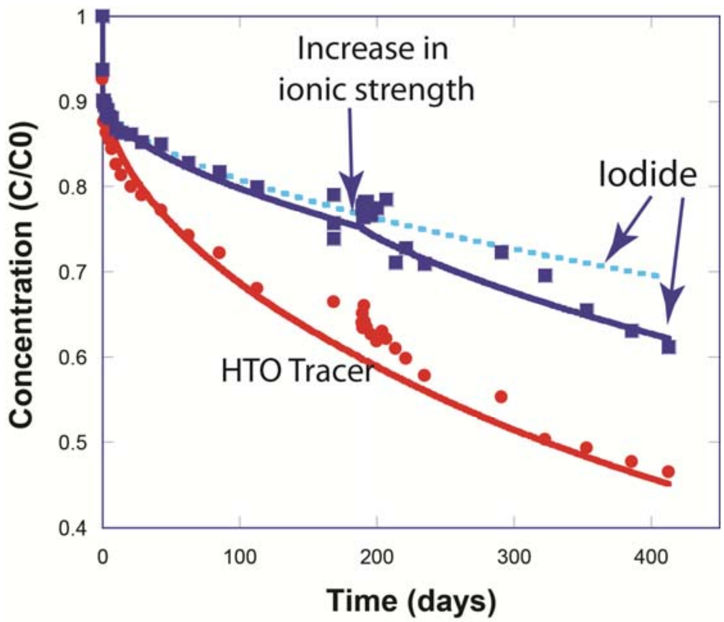


Figure 6-34. Evolution of concentration in the borehole with comparison of data (symbols) versus simulation results (solid lines) for the DR-A test through Day 412. The pale blue dashed line represents simulation results for anion diffusion where the EDL thickness and porosity is not affected by ionic strength (from Zheng et al., 2014).

6.2.3 Interpretative Analysis of Colloid Migration and Radionuclide Transport for CFM Field Experiments

In FY13 and FY14, LANL scientists conducted quantitative interpretation of radionuclide transport and colloid breakthrough from four colloid-facilitated transport tests performed as part of the CFM Project between 2008 and 2012 at the Grimsel Test Site in Switzerland (Section 3.3.1). These tests provide valuable data on how colloids released as a result of swelling and erosion of a bentonite plug will transport radionuclides through a preferred flow path such as a shear zone. Initial model interpretations conducted in FY13 (Section 2 in Wang et al., 2013) to analyze the tri- and tetravalent homologue and actinide breakthrough curves in these tests were refined in FY14, with emphasis on evaluating alternative descriptions of the desorption process of the solutes from the bentonite colloids and determining which description best explains the test observations. This activity, conducted in FY13 and FY14, is described in detail in Section 6 of Milestone Report "*Crystalline and Crystalline International Disposal Activities,*" FCRD-UFD-2014-000495 (Dittrich et al., 2014). A brief summary of the field data analysis is given below.

The interpretation of breakthrough curves in the CFM tracer tests was conducted using a semi-analytical model referred to as RELAP (REactive transport LAPlace transform) (Reimus et al., 2003) as well as a more sophisticated 2D numerical model (Reimus, 2012). RELAP uses a Fourier transform inversion method to solve the Laplace-domain transport equations in either a single- or a dual-porosity system. The model can account for diffusion between fractures and matrix, as well as linear, first-order reactions in both fractures and matrix. The very rapid execution of the model makes it ideal for the numerous simulations needed for transport parameter estimation. For each test, RELAP was first applied to fit the conservative tracer extraction breakthrough curves by adjusting the mean residence time and Peclet number in the shear zone (Peclet number is transport distance divided by longitudinal dispersivity) as well as the fractional tracer mass participation in each test. In addition to providing estimates of shear-zone transport parameters for the conservative tracers, RELAP was also used to estimate colloid transport parameters (filtration and resuspension rate constants). These estimates were obtained by assuming that the mean residence time, Peclet number, and fractional mass participation estimated for the conservative tracers also applied to the colloids, and then the filtration-rate parameters were adjusted to fit the colloid data. The resulting best-fitting parameters from RELAP were used as initial parameter estimates in a 2-D numerical model that could account for processes that RELAP does not explicitly account for. The most important of these processes were the variable injection flow rates observed in one of the field experiments and the simultaneous transport of colloids and reactive solutes in all the tests (RELAP does not account for interacting species).

It was found that once appropriate mean residence times, Peclet numbers and fractional mass participations were determined for the conservative tracer breakthrough curves in each test, and filtration parameters were determined for the colloids, the model fits to the colloid-facilitated solute breakthrough curves were sensitive mainly to the desorption-rate constants of the solutes from the colloids. The best fits to the field data were obtained when (1) the rate constants for solute adsorption to the shear-zone surfaces were large enough that the solutes rapidly adsorbed to these surfaces after they desorbed from the colloids and (2) the rate constants for solute desorption from the shear-zone surfaces were small enough that the solutes effectively did not desorb from these surfaces for the remainder of the tests. Under these conditions, the shear zone surfaces act as a fast and irreversible sink once desorption from colloids occurs. Because the tri- and tetravalent solute desorption process from colloids appeared to be so important, LANL researchers implemented into their models alternative descriptions of the solute associations with the colloids and tested these against the measured breakthrough curves from the CFM experiments. Figure 6-35 shows sample results for the model fit to the breakthrough curves for the conservative dye tracers and colloids. Overall, the simulated and measured breakthrough curves show excellent agreement, indicating the relevant processes driving colloid-facilitated transport are reasonably accounted for in the RELAP analysis, at least at the scale of the CFM test facility. As discussed in Dittrich et al. (2014), upscaling to repository scale presents further challenges.

6.2.4 Laboratory Analysis of Colloid-Facilitated Transport of Cesium by Bentonite Colloids Related to CFM

In FY15, LANL complemented the field-based colloid simulations with laboratory experiments of colloid-facilitated transport. The objective was to quantify the potential for colloid-facilitated transport of one strongly-adsorbing radionuclide, cesium (as ^{137}Cs), through a weathered fractured granodiorite system (Viswanathan et al., 2015). Cs was adsorbed to bentonite clay colloids before injection through columns packed with geologic media to provide estimates of desorption rate constants (from colloids) and other parameters that are important for performance assessment calculations. Bentonite colloids were processed from a brick of compressed bentonite from the Corijo de Archidona deposit (Almeria, Spain). This material is also called FEBEX bentonite because it was used in the FEBEX Heater Test (Section 3.3.2). Fractured and weathered granodiorite samples from the shear zone at GTS were selected as a model crystalline rock repository system because the system has been thoroughly studied, and field experiments involving radionuclides have already been conducted at this site. Working on this system provides a unique opportunity to compare lab experimental results with field-scale observations. LANL then conducted a series of batch adsorption and desorption experiments, as well as three flow-through experiments in small columns to evaluate the colloid-facilitated transport of Cs in the shear zone at the GTS. The batch adsorption and desorption experiments were conducted to evaluate the interaction of Cs with crushed fracture-fill material (FFM) from the shear zone. The experiments were performed in duplicate in polycarbonate centrifuge tubes, and a control experiment without the FFM was also conducted to allow corrections for any interaction of the Cs with the centrifuge tube walls. Column transport experiments were conducted by eluting Cs and bentonite suspensions through columns packed with FFM in the 150-355 μm size range.

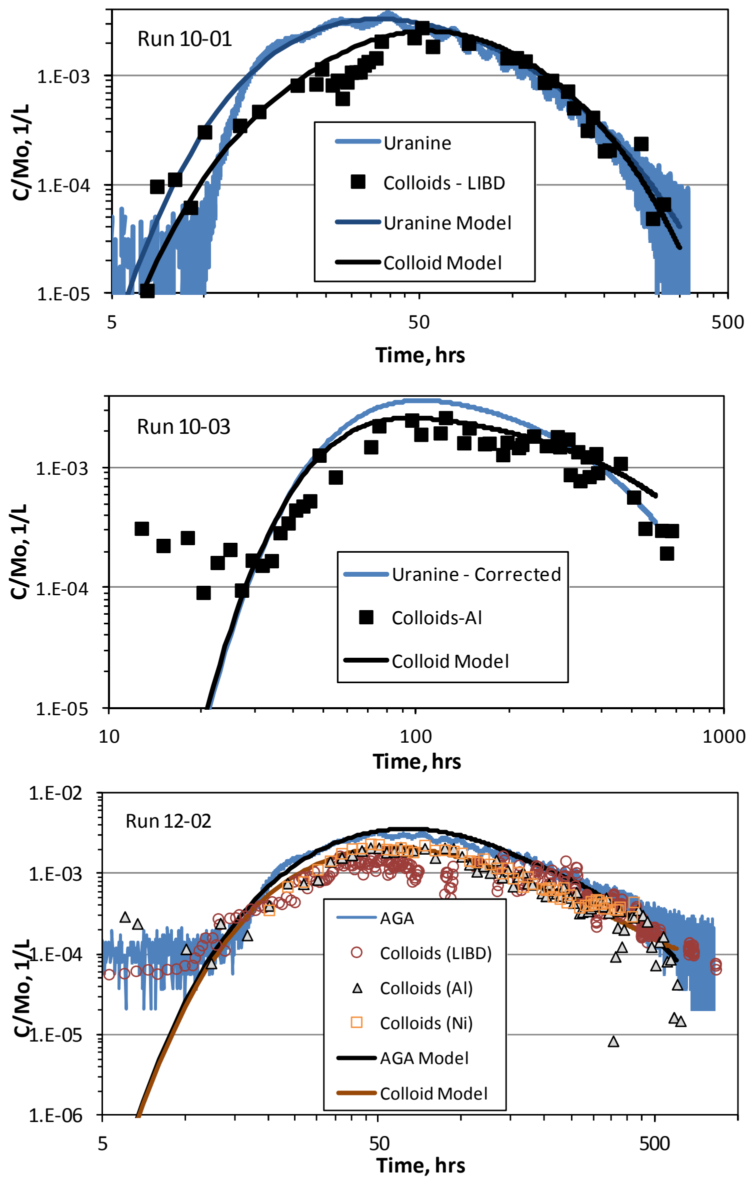


Figure 6-35. Simulated and experimental breakthrough curves for the conservative dye tracers and colloids in CFM Runs 10-01, 10-03 and 12-02. Three colloid breakthrough curves are shown for Run 12-02 because three analytical methods were used to quantify the colloid concentrations (from Dittrich et al., 2014).

Interpretative analysis was conducted as follows: The batch experiments were interpreted by simply calculating ^{137}Cs partition coefficients near the end of the experiments for either adsorption or desorption. The column modeling procedure involved first using the ^{3}HHO breakthrough curves to obtain estimates of the mean residence time and dispersivity in the columns, and then these parameters were assumed to apply to the transport of colloids and Cs through the columns. Rapid and reversible adsorption of the Cs onto the colloids was assumed based on observations that the Cs partitioning to the colloids occurred as rapidly as could be measured when ^{137}Cs-spiked suspensions were prepared. The ratios of adsorption rate constants to desorption rate constants for the Cs on both the colloids and the FFM were constrained by the partitioning observed in the batch experiments, but the rate constants themselves were allowed to vary to match the observed breakthrough curves. Figures 6-36 through 6-38 shows example results of adsorption, desorption, and flow-through experiments.

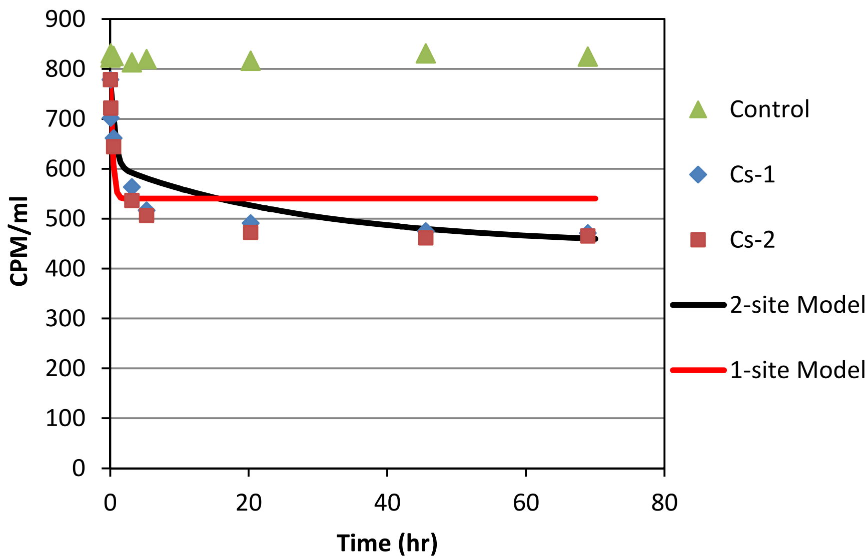


Figure 6-36. Results of batch adsorption experiment of ^{137}Cs onto fracture-fill material from GTS. The one-site and two-site model curves were generated using the best-fitting parameters for the column experiments and do not represent fits to the batch data (from Viswanathan et al., 2015).

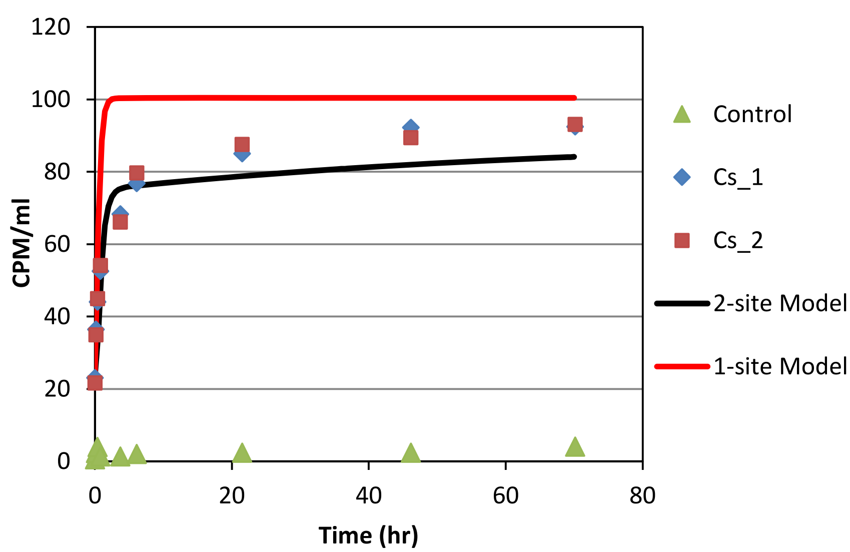


Figure 6-37. Results of batch experiment of first desorption step of ^{137}Cs from fracture-fill material from GTS. The one-site and two-site model curves were generated using the best-fitting parameters for the column experiments and do not represent fits to the batch data (from Viswanathan et al., 2015).

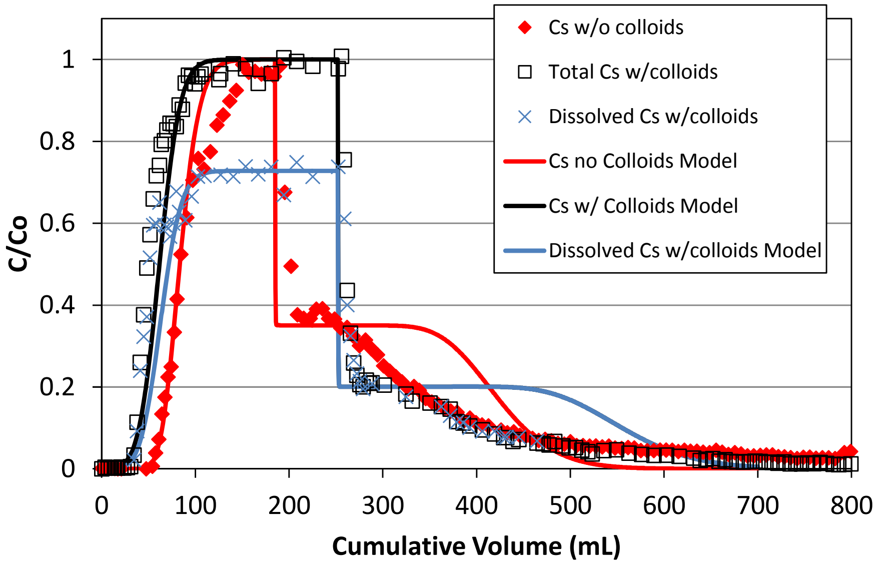


Figure 6-38. Normalized breakthrough curves of ^{137}Cs in column experiments with and without colloids in the injection pulse. Lines are model matches to the data assuming only a single type of sorption site on both the colloids and the FFM. Note that the injection pulses ended when the model curves show sudden drops in concentration. ^{3}HHO and colloid breakthrough curves are not shown, but the colloids essentially mirrored the ^{3}HHO curves and showed no evidence of any filtration (from Viswanathan et al., 2015).

Above results demonstrate how a combination of batch sorption/desorption experiments and column transport experiments could be used to effectively parameterize a model describing the colloid-facilitated transport of Cs in the Grimsel granodiorite/fracture-fill system. Cs partition coefficient estimates onto both the colloids and the stationary media obtained from the batch experiments were used as initial estimates of partition coefficients in the column experiments, and then the column experiment results were used to obtain refined estimates of the number of different sorption sites and the adsorption and desorption rate constants of the sites. The desorption portion of the column breakthrough curves highlighted the importance of accounting for adsorption-desorption hysteresis (or a very nonlinear adsorption isotherm) of the Cs on the fracture-fill material in the model, and this portion of the breakthrough curves also dictated that there be at least two different types of sorption sites on the fracture-fill material. In the end, the two-site model parameters estimated from the column experiments provided excellent matches to the batch adsorption/desorption data, which provided a measure of assurance in the validity of the model. For future work, the model developed in this study will be applied to do a forward prediction of the Cs breakthrough curve in the 2012 colloid-facilitated transport experiment at the GTS.

6.2.5 Plutonium Adsorption and Desorption Laboratory Experiments Related to CFM

In FY15, in support of the international collaboration with the CFM Project, researchers at LLNL continued their laboratory experiments and interpretation work on plutonium adsorption and desorption to bentonite. Due to its swelling properties, plasticity, ion exchange, sorption and sealing capability, bentonite is a suitable candidate for backfill material in nuclear waste repository scenarios. However, as discussed in the Sections 6.2.3 and 6.2.4, one of the concerns with the use of bentonite is that it can form colloidal particles, which may enhance the migration of radionuclide species (Geckeis et al., 2004; Kersting et al., 1999). As a result, radionuclide (including Pu) adsorption to mineral colloids has been the subject of considerable research. In contrast, desorption reactions have been far less well studied. The aim of LLNL's FY15 activities has been two-fold: (1) to provide information on Pu adsorption/desorption to FEBEX bentonite, a backfill material used at the Grimsel Test Site, and (2) to determine if the linearity observed for Pu(V) sorption to a pure clay mineral is replicated for Pu(IV) sorption to a multicomponent clay rock. To this extent, the sorption behavior of Pu(IV) to FEBEX bentonite was examined in laboratory experiments across a wide range of initial concentrations (10^{-7} – 10^{-16} M) over a 120 d period. In addition, LLNL performed long-term (10 month) adsorption experiments with Pu(V) to better constrain the slow apparent rates of reduction on bentonite. The experimental setup and results are described in Milestone Report "*Progress Report on FY15 Crystalline Experiments,*" M4FT-15LL0807052 (Zavarin et al., 2015). LLNL's experiments demonstrate the control that the montmorillonite in bentonite exerts on the adsorption behavior of Pu, provide long-term adsorption data useful for the interpretation of colloid transport experiments at the Grimsel test site, and validate the extrapolation of Pu(IV) experiments performed at concentrations of 10^{-10} M Pu to concentrations typically found in the environment at timescales relevant for groundwater transport.

6.3 Characterization and Monitoring Techniques

6.3.1 R&D Cooperation with KAERI at the KURT URL

As part of ongoing bilateral collaboration between DOE and the Republic of Korea (Section 4.1), researchers at SNL have developed a multi-year plan for joint field testing and modeling to support the study of high-level nuclear waste disposal in crystalline geologic media. The work for FY15 focused on two tasks: (1) streaming potential (SP) testing to better understand groundwater flow and transport, and (2) technique development for *in situ* borehole characterization.

6.3.1.1 R&D Cooperation with KAERI Regarding Streaming Potential

The SP method is a geophysical technique that is sensitive to the movement of groundwater in real time. The method is based on the fact that the streaming of water through pores and fractures in the ground can produce a natural electrical potential (called streaming potential) along the flow path. Therefore, unlike other geophysical methods, there is a direct relation between SP signal and groundwater flow. The objective of the collaborative R&D between SNL and KAERI is to evaluate whether the SP method can also be used to estimate solute transport characteristics of an aquifer. In FY15, the joint research team conducted tracer tests under steady-state groundwater flow condition with recording SP signals (Wang et al., 2015). An acrylic tank was filled with medium to coarse-grained sand and infiltrated with water (Figures 3-39 and 3-40). The team then tried to detect the changes in SP signals due to injection and transport of tracer.

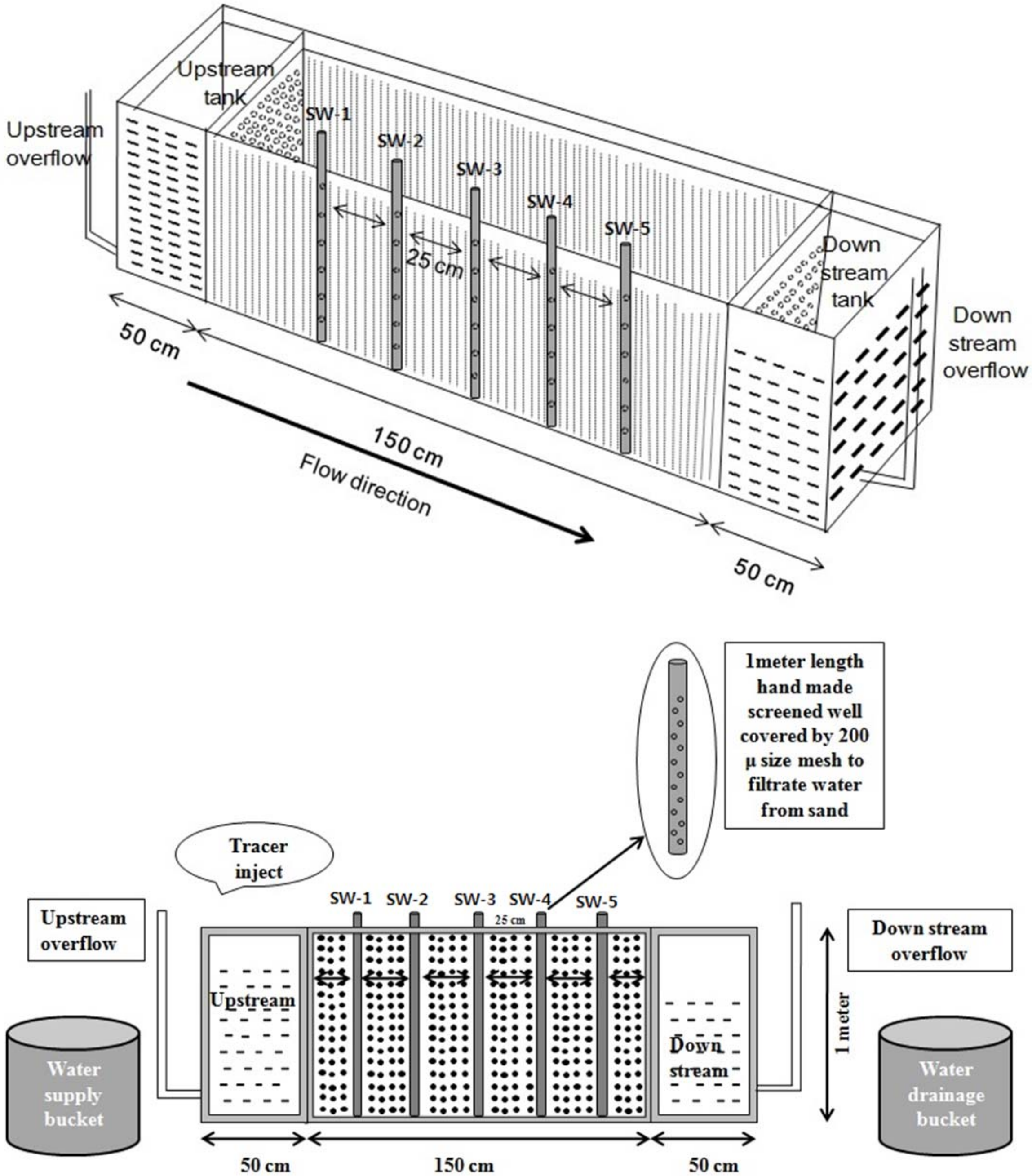


Figure 6-39. Design of sandbox (from Wang et al., 2015)

Figure 6-40. Full setup of a sandbox experiment (from Wang et al., 2015)

Tracer tests were performed in the sandbox with the help of peristaltic pump, and tracer samples were collected from the same interval of five screened wells in the sandbox. During the tracer test, SP signals resulting from the distribution of 20 nonpolarizable electrodes were measured at the top of the tank by a multichannel meter. The results showed that there were changes in the observed SP after injection of the tracer, which indicated that the SP was likely to be related to the solute transport. However, further testing is needed to confirm these preliminary results.

6.3.1.2 R&D Cooperation with KAERI Regarding Deep Borehole Disposal

As mentioned above, KAERI and SNL are collaborating on a second task: technique development and demonstration for *in situ* borehole measurements. This task is a jointed effort between the UFD deep borehole disposal work package and the crystalline disposal R&D work package. In FY15, SNL finalized a new contract with KAERI on a collaborative work the development of in-situ hydrological and geochemical measurements in boreholes. The goal of this collaborative work it to initiate an actual field test at the KURT site for the development of in-situ measurement techniques in boreholes (Wang et al., 2015).

6.3.2 Collaboration with COSC Project in Sweden on Deep Borehole Disposal

COSC stands for "Collisional Orogeny in the Scandinavian Caledonides" and is a scientific deep drilling project with the primary objective of resolving some key issues in orogenesis, but also with geophysical, hydrological, geothermal, microbiologic, and geochemical measurement goals. The project is centered on the drilling of two deep boreholes (each to depth of 2.5 km) into crystalline rock in Sweden. One of the holes (COSC-1) was drilled last year and another will be drilled in 2017. Core was collected from the first borehole COSC-1 with over 99% core recovery. In FY15, LBNL scientists started collaborating with the COSC project as part of the UFD campaign's deep borehole activity. This is to take advantage of the data and experiences in drilling and testing in the first 2.5-Km COSC-1 borehole that was completed on 26 August 2014. In the drilling of COSC-1, the Swedish scientists kept a good record of (1) drilling experience with more than 99% core recovery; (2) pre-drilling and post-drilling seismic and other geophysical surveys, (3) borehole geophysical logs, (4) core handling procedure and immediate on-site measurement on recovered cores, (5) systematic XRF measurement on all cores at 10 cm intervals for key chemical compositions, and (6) downhole SGR logging to determine U, Th and K content all along the borehole.

COSC provides a leveraged opportunity for DOE to test deep borehole characterization techniques that could be used for the planned UFD deep borehole, such as the hydrologic logging using a method called the flowing fluid electrical conductivity (FFEC) log that was developed at LBNL (Figure 6-41). The FFEC logs can be used to identify locations of hydraulically active zones at decimeter (10-cm) resolution in the borehole. In the summer of 2014 during the drilling period, COSC already conducted preliminary FFEC logging, successfully identifying five hydraulically conductive zones along the borehole depth from 300m to 2500m and providing estimates of their transmissivities (Figure 6-42). The experience with the FFEC logging conducted in Sweden can be very important when conducting similar field monitoring in deep borehole demonstration project currently planned in the US.

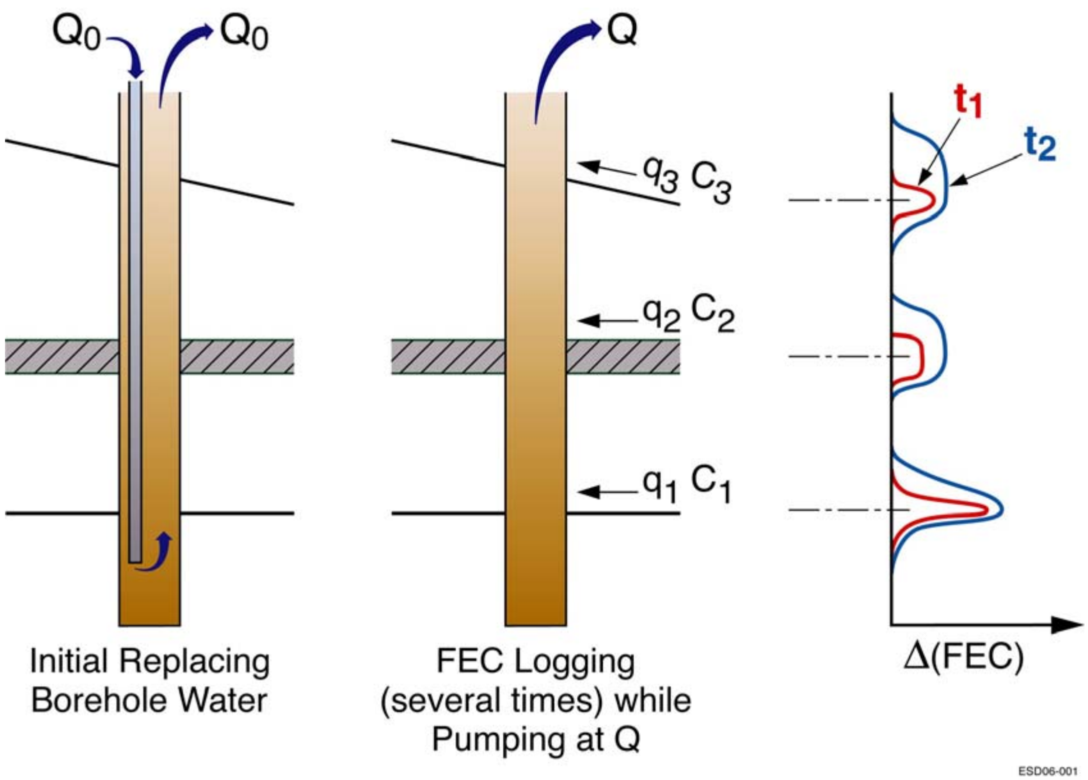


Figure 6-41. Schematic depiction of FFEC logging method for detection of hydraulically conductive inflow zones into the borehole

In FY15, under the COSC collaboration, LBNL studied and analyzed existing data from the COSC-1 borehole as a case study, with the goal to develop a better understanding of what information can be obtained from core and borehole measurements and what is the deep subsurface environment in granitic rocks in the context of nuclear waste disposal. LBNL and COSC scientists are now in the process of conducting a longer-term repeat FFEC logging campaign at COSC-1 to improve on the preliminary measurements. Because of operational limitations during the drilling period, the preliminary logs data are limited and their analysis involved some uncertainties. The improved FFEC log data will be analyzed at LBNL. The field activities are integrated with a laboratory measurements program at LBNL. LBNL has obtained water samples and core samples around both flowing and non-flowing fractures for laboratory testing at LBNL. These are full-round (diameter of 3 or 4 inch), vertically-oriented cores up to 8 inches long (Figure 6-43). The laboratory measurements program has three parts: (i) chemical analysis of water samples from the eight identified flow zones at COSC-1 borehole; (ii) analyses of rock matrix and fracture minerals of core samples by optical mineralogy in thin sections to determine how fracture mineralogy differs from the bulk rock and what are the differences in diagenetic alteration between hydraulically active fractures and fractures without measurable hydraulic conductivity, and (iii) measurement of fracture permeability of cores from the eight flow zones as a function of controlled stress. These laboratory permeability measurements will be compared with in-situ determinations from the detailed FFEC logging. Further, an integrated study will be made of these results, together with other data from the COSC project (temperature, dipmeter, sonic, acoustic televiewer, rock resistivity, spectral gamma ray, and magnetic susceptibility logs, etc.) which will be made available to us, to understand and evaluate the hydraulic structure, permeability variation, and geochemical distribution in the deep subsurface environment in granitic rock, in the context of their suitability for nuclear waste disposal.

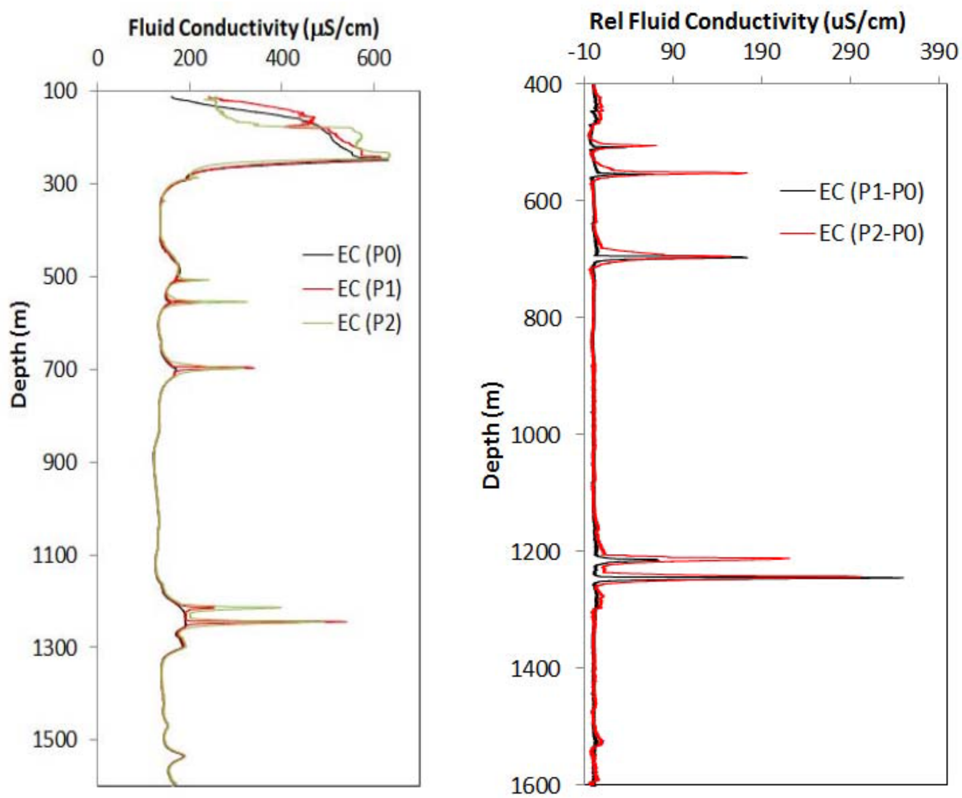


Figure 6-42. Fluid Electric Conductivity measured in the preliminary FFEC logging. Left: absolute values from P0 (no pumping) and P1 and P2 (two times after pumping started). Right: changes between P1 and P0, and P2 and P0.

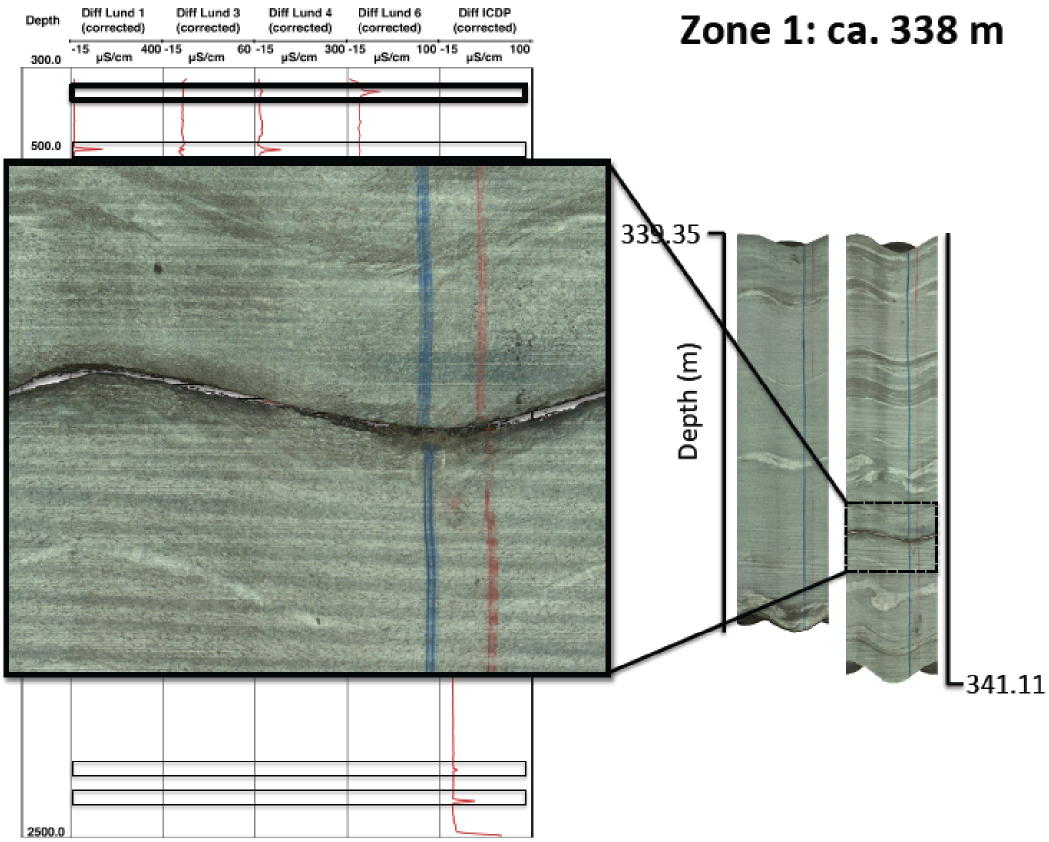


Figure 6-43. Core sample obtained for one of the five hydraulically conductive inflow zones with a distinct fracture zone intersecting the borehole

7. BRIEF STATUS OF OTHER INTERNATIONAL COLLABORATION ACTIVITIES

This section provides brief descriptions of ongoing international collaboration activities that are not directly associated with access to field data or participation in URL field experiments. As with the remainder of this report, the focus here is on active collaboration in specific R&D projects, not on conferences, meetings, or other types of information exchange.

7.1 Collaborative Salt Repository Research with Germany

There are ongoing collaborative efforts between scientists from the U.S. and Germany regarding salt as a host rock for radioactive waste. These collaborative efforts focus on fundamental topics such as thermomechanical behavior of salt, plugging and sealing, the safety case, and performance assessment, and are aimed at advancing the basis for disposal of heat-generating nuclear waste in salt formations. In addition, the topic of operational safety was introduced as a new collaborative topic in FY15. Two salt conferences were held to further these collaborations: the 5th US/German Salt Workshop (Hansen et al., 2015), held September 8-10, 2014 in Santa Fe, New Mexico; and the 4th Nuclear Energy Agency (NEA) Salt Club Meeting, held February 25, 2015 in Paris, France. Details of the collaborations in each of these areas are summarized below (mainly based on Milestone Report "*Status of UFD Campaign International Activities in Disposal Research at SNL*," FCRD-UFD-2015-000713, McMahon, 2015).

Design and Operational Safety

The serious operational events at WIPP in 2014 provided sharp focus and tangible reality to the topic of operational safety. Workshop participants gained deeper appreciation for the seriousness of operational safety and the complexity involved with recovery from off-normal events. Design of a salt repository for high-level waste and spent nuclear fuel takes into account retrievability and safety requirements. Examples provided at the 5th US/German Workshop included:

- In 2010, the Bundesministerium für Umwelt (German Federal Ministry for the Environment, Nature Conservation and Nuclear Safety) issued the new *Safety Requirements Governing the Final Disposal of Heat-Generating Radioactive Waste*. The safety requirements focus on retrievability and make it a strict licensing requirement. According to the safety requirements, retrievability is considered as the planned technical option.
- A very recent and important development is the increasing relevance of probabilistic approaches in the regulation of geologic repositories. The shift from deterministic to probabilistic approaches is clearly exemplified in the US DOE nuclear facility safety analysis (WIPP Documented Safety Analysis) and the Yucca Mountain License Application. For the Yucca Mountain Project probabilistic requirements have even been formalized in the U.S. safety regulation (10 CFR Part 63). It can be seen that operational safety analysis is changing, at the same time that safety experience is accumulating at existing facilities. Especially for new systems and technologies, probabilistic approaches provide important supplements for safety demonstration. Nevertheless, since probabilistic approaches for large-scale systems are yet under development it is of vital importance to facilitate an international exchange in order to avoid diverging methodologies, respectively to build up confidence in probabilistic approaches.

Geomechanical Issues

Ongoing collaborations between US and German salt researchers include testing on all scales, advanced thermal-mechanical modeling and benchmarking, and seal system performance, to name a few. Specific collaborations in FY15 included:

- Investigations of the mechanical response and evolution of the salt underground initiated by excavation, including ongoing geomechanics matters pertaining to room closure.
- Code benchmarking of salt constitutive modeling and implementation using large modern computational frameworks.
- Continued collaboration in laboratory and field testing and geomechanical modeling. This work has ensured validated and verified computational capabilities for both bedded and domal salt are being developed and parameterized.
- Lessons learned from the Gorleben site (Vorläufige Sicherheitsanalyse Gorleben or VSG)
- Plugging and sealing studies

Underground Research Laboratory Developments (URL)
In collaboration, US and German researchers have reviewed and evaluated thermally driven processes in salt disposal and identified key technical areas in which to prioritize resources. The goal for disposal research in salt is to provide sufficient technical information to license a repository successfully. The necessity or utility of a salt underground laboratory is to be evaluated in the context of an overall research agenda that supports a license application. In both advanced programs and also in the less advanced ones URLs are considered to be indispensable especially to perform experiments and demonstration activities under repository like conditions. Specific activities in FY15 included:

- Discussion of the need for a salt URL (including bedded and/or domal salt)
- Identification of a generic research strategy and proposed testing activities for a salt URL.
- Discussion of the use of a URL or other mined salt formation for experimental activities that could capture the early evolution of a salt excavation (e.g., examine the initial, undisturbed conditions, the evolutionary changes imparted by excavation, and the boundary conditions extant when field activities are undertaken).

Safety Case for Heat-Generating Waste Disposal in Salt
Specific collaborations in FY15 included:

- Subject matter experts from the US and Germany are in the process of compiling a comprehensive Features, Events, and Processes (FEPs) catalogue for disposal of heat-generating waste in salt (Freeze et al. 2014).
- SNL has developed a generic safety case for disposal of heat-generating waste in bedded salt. Collaborators discussed elements of the safety case including handling uncertainties and the qualitative contribution of analogues. This progress along with Germany's preliminary safety analysis for the Gorleben site (Vorläufige Sicherheitsanalyse Gorleben or VSG) provide a strong technical basis for a safety case for salt disposal of heat-generating nuclear waste.
- SNL has developed a salt knowledge archive.
- Far-field hydrogeologic modeling, with applicable porous and fractured media flow.
- Exploring public outreach initiatives implemented successfully in other countries to help frame a societal strategy.

7.2 Thermodynamic Database Evaluations

Thermodynamic data are essential for understanding, evaluating, and modeling geochemical processes, such as speciation solubility, reaction paths, or reactive transport. The data are required to evaluate both equilibrium states and the kinetic approach to such states. However, thermodynamic databases are often limited and do not span the range of conditions that may exist under the various generic repository scenarios (salt, deep borehole, etc.). For example, previously developed thermodynamic data overstate the stabilities of smectites and illites. While this is adequate for both tuff and salt host rock, the databases have some deficiencies with respect to other repository designs, such as those in clay/shale, or those that include a clay/bentonite buffer. Data that continue to come out of the NEA thermochemical database review program were not incorporated into the previous DOE thermodynamic databases. Furthermore, NEA data are also limited and do not account for pressure extrapolations applicable to deep borehole repositories. Ion exchange data and surface complexation processes are also lacking in most current thermodynamic databases.

Scientists at LLNL have collaborated with the international research community to improve thermodynamic databases and models that evaluate the stability of EBS materials and their interactions with fluids at various physico-chemical conditions relevant to subsurface repository environments. The development and implementation of equilibrium thermodynamic models are intended to describe chemical and physical processes such as solubility, sorption, and diffusion. As part of this work, LLNL scientists have continued participating in the NEA Thermochemical Database (TDB) Project (see Section 3.5.3). Furthermore, LLNL has revised previously developed thermodynamic databases and expanded them to cover the needs of the repository types currently under consideration by UFD (i.e., clay, granite, deep borehole). In another collaborative effort, LLNL scientists have worked with colleagues from the Helmholtz Zentrum Dresden-Rossendorf in Germany to develop improved thermodynamic data for high-ionic-strength conditions and surface-complexation models. Progress made on these tasks is documented in the Milestone Report "*Thermodynamic and Sorption Data FY15 Progress Report*," M4FT-15LL0806062 (Zavarin et al., 2015).

8. SUMMARY

Active collaboration with international programs, initiatives, or projects is very beneficial to UFD's disposal research program, providing access to the decades of experience that some international programs have gained in various disposal options and geologic environments. The first part of this report discusses opportunities for active international collaboration, with focus on those opportunities that involve field experiments in international URLs. Section 3 contains a summary of currently existing international opportunities resulting from DOE's formal "membership" in international collaborative initiatives, such as the DECOVALEX Project, the Mont Terri Project, the Colloid Formations and Migration Project, the FEBEX-DP Project, and the SKB Task Forces. Benefits of DOE participation include (1) access to experimental data from many past, ongoing, and future *in situ* tests conducted in several URLs in different host rocks, (2) active research participation in international groups that conduct, analyze, and model experiments, and (3) the opportunity to conduct own experiments in international URLs. Additional cooperation possibilities are discussed in Section 4; these comprise bilateral collaborations options with international disposal programs.

With many collaboration opportunities available to UFD, the campaign in FY12 started a planning exercise to identify the most relevant and promising opportunities, and to select and initiate several cooperative R&D activities that align with its goals and priorities. The following criteria were applied: (1) Focus on activities that complement ongoing disposal R&D within UFD, (2) Select collaborative R&D activities based on technical merit, relevance to safety case, and cost/benefit, and strive for balance in terms of host rock focus and repository design, (3) Emphasize collaboration that provides access to and/or allows participation in field experiments conducted in operating underground research laboratories not currently available in the U.S. (i.e., clay, crystalline), (4) Focus on collaboration opportunities for active R&D participation.

Since 2012, UFD scientists have participated in various collaborative projects to address high-priority R&D challenges related to near-field perturbation, engineered barrier integrity, flow and radionuclide transport, integrated system behavior, and method development for characterization and monitoring. The second part of this report provides an overview of this collaborative R&D portfolio and explains how UFD scientists benefit from collaboration with international peers. Section 5 describes the planning process that led to the selection of specific activities. Section 6 then gives a detailed description of projects that make use of international field experiments, and Section 7 briefly mentions other active cooperation projects. Overall, this report attests to the fact that DOE/UFD has in a very short time frame developed a balanced portfolio of international research collaborations that have already led to substantial technical advances (i.e., several science and engineering tools developed in UFD were tested in comparison with data from international experiments). UFD scientists have utilized data and results from laboratory and field studies that have been and are being conducted with millions of R&D investments provided by international partners. UFD's advanced simulation models are being verified and validated against these experimental studies, providing a robust modeling and experimental basis for the prediction of the complex processes defining the performance of a multibarrier waste repository system. Comparison of UFD model results with other international modeling groups, using their own simulation tools and conceptual understanding, enhanced confidence in the robustness of predictive models used for performance assessment. And the possibility of linking model differences to particular choices in conceptual model setup provides guidance into "best" modeling choices and understanding the effect of conceptual model variability. Promising opportunities exist for further expansion of the international program.

In FY15, UFD re-evaluated its international research portfolio, in a process similar to the initial planning phase in 2012. As research priorities change and new opportunities for collaboration develop, one objective was to reassess the relevance of ongoing activities in light of new possibilities for cooperation. As a result, UFD decided in FY15 to end its participation in the CFM Project because of its relatively narrow focus and relatively high participatory cost. In contrast, all other international collaborative projects described in Section 4 are considered extremely valuable and will continue in future years. The joint R&D with international researchers and the access to relevant data/experiments from a variety of URLs and host rocks have helped UFD researchers to significantly improve their understanding of the current technical basis for disposal in a range of potential host-rock environments and has contributed to testing and validating predictive computational models for evaluation of disposal-system performance in a variety of generic disposal-system concepts.

In the future, UFD will also evaluate whether its international collaboration focus should move from a mostly participatory role in ongoing *in situ* experiments conducted by other nations, to a more active role in developing its own experimental program in international URLs. Some collaborative initiatives like the Mont Terri Project provide their partner organizations with the opportunity of conducting their own experimental work and inviting other partners to join. This option would allow the U.S. disposal program to perform *in situ* field work in representative host rocks (clay, crystalline), even though there are currently no operating underground research laboratories in the U.S.

9. ACKNOWLEDGMENTS

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