Title

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Publication Date

2024-09-30

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Lawrence Berkeley National Laboratory
Report LBNL-2001608

September 30, 2024

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International Collaboration Activities in Geologic Disposal Research: FY24 Progress Report

Spent Fuel and Waste Disposition

Prepared for
U.S. Department of Energy
Office of Nuclear Energy
By Lawrence Berkeley National Laboratory

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September 30, 2024

LBNL-2001608

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NFCSC DOCUMENT COVER SHEET[1]

Name/Title of Deliverable/Milestone/Revision No.	International Collaboration Activities in Geologic Disposal Research: FY24 Progress Report / M2SF-24LB010307012
Work Package Title and Number	Disposal Research International Coordination – LBNL / SF-24LB01030701
Work Package WBS Number	1.08.01.03.07
Responsible Work Package Manager	Jens Birkholzer [signature] (Name/Signature)
Date Submitted	09/30/2024

Quality Rigor Level for Deliverable/Milestone[2]	☐ QRL-1 ☐ Nuclear Data	☐ QRL-2	☒ QRL-3	☐ QRL-4 Lab QA Program[3]

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☒ DOE Order 414.1 ☐ NQA-1 ☐ Other

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ABSTRACT

This report describes the FY24 status of international collaboration regarding geologic disposal research in the Office of Spent Fuel and Waste Science and Technology (SFWST) in the Department of Energy's (DOE) Office of Nuclear Energy (NE). The mission of SFWST is to provide confidence in the safe long-term management of the nation's spent nuclear fuel and high-level radioactive waste by reducing uncertainty and advancing technology for extended storage, transportation, and geologic disposal.

High-Level Objective of International Collaboration in Geologic Disposal Research

Since 2012, Lawrence Berkeley National Laboratory (LBNL) has coordinated the SFWST efforts to advance active collaboration with several international geologic disposal programs across the world. The joint research activities with international programs, initiatives, and projects are beneficial to SFWST's disposal research program because they: (1) provide first-hand access to the decades of experience of our international partners gained in investigations of various disposal options in geologic environments; (2) give SFWST scientists a large library of experimental data from many past and ongoing *in-situ* tests conducted in several international underground research laboratories (URLs) in different host rocks; (3) provide a framework for active peer-to-peer research participation in international groups that conduct, analyze, and model performance-relevant processes; and (4) open the door to jointly conducting SFWST *in-situ* experiments in international URLs not available in the U.S. Last not least, international collaboration allows the SFWST Campaign to benefit from substantial international investments in research facilities (such as underground research laboratory testing and modeling) and achieve cost savings via joint funding of expensive field experiments.

Status of International Collaboration

Over the past decade, SFWST's International Disposal Research and Development (R&D) Program has established formal collaboration agreements with multiple international initiatives and various international partners, and national lab scientists associated with SFWST have conducted many specific collaborative R&D activities that align well with its R&D priorities. Formal partnerships in collaborative initiatives, such as the Mont Terri Project (since 2012), the DECOVALEX Project (since 2012), the Colloid Formation and Migration Project (CFM) (2012 – 2015), the FEBEX Dismantling Project (2015 – 2018), the SKB Task Forces (since 2014), and the HotBENT Project (since 2018), have allowed access to collaborative research with a focus on field experiments in international URLs. Other multinational initiatives, such as several Nuclear Energy Agency (NEA)-coordinated activities, have provided valuable opportunities for information exchange and data assessment. Additional opportunities for multinational collaboration exist: For example, SFWST just instituted a technical partnership with the EURAD-2 European Commission collaborative research program which initiated a new round of repository R&D work for a 5-year period from 2024 through 2029. The SFWST campaign has also explored direct bilateral opportunities for active research collaboration, with institutions from Germany, Republic of Korea, Sweden, Israel, France, Japan, Belgium, Finland, Czech Republic, and China. Some of these opportunities (e.g., with Germany, Republic of Korea, Sweden, Israel, and France) have resulted in close bilateral research activities between SFWST scientists and their international counterparts; the others provide opportunities for active research collaboration in the future.

International collaboration opportunities and international activities form a considerable portion of the SFWST campaign's disposal research program, specifically in key disposal research areas such as the Engineered Barrier System (EBS), Crystalline, Argillite, and Salt Work Packages, and more recently also in the Geologic Disposal Safety Assessment (GDSA) Work Packages. In a balanced portfolio, international collaboration activities address important research areas such as engineered barrier integrity, near-field perturbations, radionuclide transport, integrated system behavior, performance assessment, site characterization and monitoring approaches.

Accomplishments

The focus on international collaboration has allowed for deep engagement of U.S. researchers with the international waste disposal R&D community in terms of best practices, new science advances, state-of-the-art simulation tools, site characterization and monitoring approaches, lessons learned, etc. Accomplishment highlights are listed below:

- The joint R&D with international researchers, the worldwide sharing of knowledge and experience, and the access to data for field and laboratory experiments from a variety of URLs and host rock have helped SFWST researchers significantly improve their understanding of the current technical basis for disposal in a range of potential host-rock environments.
- SFWST 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.
- Advanced simulation models have been verified and validated against these experimental data, providing a robust modeling and experimental basis for the prediction of the complex processes defining the performance of a multi-barrier waste repository system.
- International scientists have contributed to the analysis and interpretative modeling of laboratory or field studies performed by SFWST, such as the HotBENT Lab Experiments and the BATS field experiments.
- Comparison of model results with other international modeling groups, using their simulation tools and conceptual understanding, has enhanced confidence in the robustness of predictive models used for performance assessment.
- The possibility of linking model differences to conceptual model setup has provided valuable guidance into "best" modeling choices and understanding the effect of conceptual model selection on prediction uncertainty. Such advances in the ability to make long-term predictions of complex coupled thermo-hydro-mechanical-chemical (THMC) and flow and transport processes contribute directly to improved post-closure performance assessments (PA) models.
- Access to international field testing has provided an opportunity to develop, test, and demonstrate new methods and workflows for site characterization and monitoring of deep geological disposal.
- International collaboration has provided valuable opportunities for recruiting/training/educating junior staff, a promising avenue for developing a next-generation workforce of disposal scientists.

Future Work

Going forward, international collaboration will remain an important cross-cutting campaign activity within the SFWST campaign. SFWST's international research portfolio has evolved and will continue to evolve as the campaign's priorities change and new opportunities emerge. The campaign routinely reviews, assesses, and develops such opportunities in close integration with international partners, evaluates the technical merit and alignment with SFWST priorities, and revises the portfolio of international R&D activities as appropriate. Given its importance within the overall portfolio of disposal research activities, any such planning and prioritization is done in tight integration with all other disposal research work packages, e.g., the host-rock-specific research portfolios, the EBS research portfolio, and the performance assessment research portfolio. This report identifies several additional opportunities for international collaboration that the campaign may consider going forward, including new international field experiments as well as opportunities related to international siting approaches and site characterization practices.

EXECUTIVE SUMMARY

Background and Main Objectives

This report describes the FY24 status of international collaboration regarding geologic disposal research in the SFWST Campaign. Since 2012, in an effort coordinated by LBNL, SFWST has advanced active collaboration with several international geologic disposal programs worldwide. Such collaboration has allowed the SFWST Campaign to benefit from a deep knowledge base regarding alternative repository environments developed over decades. It has provided a framework for active peer-to-peer research participation in international groups that conduct, analyze, and model performance-relevant processes. Via international collaboration, the SFWST Campaign also benefits from substantial international investments in research facilities (such as URL testing and modeling). It achieves cost savings via joint funding of expensive field experiments. To date, SFWST's International Disposal R&D Program has established formal collaboration agreements with multiple international initiatives and various international partners, and national lab scientists associated with SFWST have conducted many specific collaborative R&D activities that align well with its R&D priorities. Guiding principles for the selection of collaboration options and activities have been as follows:

- Focus on activities that align with the strategic direction of the SFWST campaign and complement ongoing disposal R&D (e.g., testing the science and engineering tools developed in SFWST in comparison with international experiments).
- Select collaborative R&D activities based on technical merit, relevance to safety case, and cost/benefit, and strive for balance regarding host rock focus and repository design.
- Emphasize collaboration that provides access to and/or allows for participation in field experiments conducted in operating underground research laboratories in clay, crystalline, and salt host rock, which are not currently available in the U.S.
- Focus on collaboration opportunities for active R&D participation of U.S. researchers and close collaboration with international scientists on specific R&D projects relevant to both sides

Key Issues Tackled in Current and Planned Portfolios

The current work conducted within international activities centers on the following key research questions:

- *Engineered Barrier Integrity:* What is backfills and seals' long-term stability and retention capability? Can bentonite be eroded when in contact with water from flowing rock fractures? How relevant are interactions between engineered and natural barrier materials, such as metal-bentonite-cement interactions? Is gas pressure increase or gas migration a concern for barrier integrity?
- *Near-Field Perturbation:* How important are thermal, mechanical, and other perturbations to a host rock (such as argillite/clay/shale, crystalline rock, and salt), and how effective is healing or sealing of the damage zone in the long term? How reliable are predictive models for the strongly coupled THMC (thermal-hydrological-mechanical-chemical) behavior of clay and salt formations?
- *Flow and Radionuclide Transport:* How does high temperature affect the diffusion and sorption characteristics of clay materials (i.e., considering the heat load from dual-purpose canisters)? What is the potential for enhanced transport with colloids? Can transport in diffusion-dominated formations (i.e., clay, bentonite, salt) and advection-dominated systems (i.e., fractured granite) be predicted with confidence?

- *Integrated System Behavior, Performance Assessment, and Site Characterization:* Can the early-time behavior of an entire repository system, including all engineered and natural barriers and their interaction, be measured and demonstrated? Can this integrated behavior be reliably predicted? Are the planned construction and emplacement methods feasible? Which characterization and monitoring methods are suitable for site selection and performance confirmation? How reliable are performance assessment models?

Collaboration Opportunities Provided by International Initiatives (Section 3 of this report)

Since 2012, SFWST has joined several multinational collaboration initiatives as a formal partner and has established a balanced portfolio of selected R&D projects collaborating with international peers. Below. We provide short summaries of active collaboration agreements (Mont Terri Project, DECOVALEX Project, HotBENT Project, and SKB Task Forces) and briefly describe partnerships that have officially ended but continue to provide opportunities for informal collaboration (FEBEX-DP Project and CFM Project).

Mont Terri Project (since 2012)

The Mont Terri Project is an international research partnership (currently 22 partners) for the characterization and performance assessment of a clay/shale formation. The partnership provides open access to an existing URL in Switzerland, the Mont Terri URL. Partner organizations can conduct experiments in the URL, participate in experiments conducted by others, and have access to all project results from past and ongoing efforts. In the current phase, the Mont Terri Project comprises about 40 separate experiments relevant to all phases in the lifetime of a repository. The annual budget for the *in-situ* work amounts to several million U.S. dollars, complemented by the partners' interpretation, analyses, and modeling work. The U.S. Department of Energy (DOE) joined the Mont Terri Project in July 2012. Since then, SFWST researchers have engaged in projects ranging from large-scale heater tests to damage zone characterization, diffusion, engineered barrier material interaction, and fault slip experiments. A significant extension of the Mont Terri URL has been undertaken in 2019-2020, providing significantly more space for new experiments. This extension ensures the long-term future of the Mont Terri Project.

DECOVALEX Project (since 2012)

The DECOVALEX Project (DEvelopment of COupled Models and their VALidation Against EXperiments) is an international research collaboration and model comparison activity for coupled process simulations in geologic repository systems (currently 18 partners). The project has been active and running for more than 30 years and is aimed at developing modeling test cases based on experimental data sets from international URLs. Typically, these experimental test cases are proposed by one of the project's partners and collectively studied and modeled by all DECOVALEX participants. During this reporting year, DOE scientists finalized their participation in a broad range of relevant modeling tasks associated with the most recently completed DECOVALEX Project phase, referred to as DECOVALEX-2023, which was initiated in early 2020 and ended in December 2023. These tasks included *in-situ* tests on thermal and gas fracturing in argillite, gas migration in bentonite, a full-scale demonstration test in a clay host rock, a full-scale engineered barrier experiment, and a more fundamental task involving laboratory experiments fluid flow, shear, thermal and reaction processes. SFWST scientists also served as task leads for two additional tasks, one focusing on brine migration in heated salt, and one on performance assessment. The currently active DECOVALEX Project phase, or DECOVALEX-2027, started in the Spring of 2024 and will run through the end of 2027. SFWST scientists are deeply engaged in this new phase, again leading two modeling tasks and participating in seven of the eight tasks.

Grimsel Test Site Projects (since 2012)

The Grimsel Test Site (GTS) is a URL situated in sparsely fractured crystalline host rock in the Swiss Alps. GTS was established in 1984 as a center for underground R&D supporting a wide range of disposal research projects related to crystalline rock and EBS. SFWST was a partner in the CFM Project at GTS from 2012 through 2015, participated in the FEBEX-DP from 2015 to its official close in 2018, and is currently one of several international partner organizations engaged in the high-temperature HotBENT experiment (since 2018). Participation in these collaborative projects required separate agreements between the GTS operator Nagra and its partners.

– The CFM Project is an international research project investigating colloid formation, bentonite erosion, migration, and colloid-associated radionuclide transport. The project conducts radionuclide migration experiments in a fracture shear zone in the GTS, complemented by laboratory and modeling studies. DOE joined the CFM Project in August 2012 but ended its official membership in 2015. There are no SFWST activities directly related to CFM. Still, SFWST researchers are currently performing experiments to study bentonite clay erosion, coagulation, and flocculation, and simulated fracture clogging behavior under controlled conditions. This work is loosely connected with the *In-situ* Bentonite Erosion Test (i-BET) experiment conducted under the umbrella of the CFM Project.

– The Full-scale Engineered Barriers EXperiment (FEBEX) was a full-scale *in-situ* heater test focusing on bentonite backfill in a crystalline host rock. The test started at the Grimsel Test Site in 1997 and ended in 2015 after 18 years of operation at a bentonite temperature of up to 100°C. A related international collaboration project, referred to as the FEBEX Dismantling Project (FEBEX-DP), was initiated in 2015 and aimed to carefully dismantle the test site, perform a post-mortem analysis of engineered and natural barrier components, and conduct a joint study of the integrity of these barriers. DOE joined the FEBEX-DP Project as one of the initial partners. Though the project officially ended in 2018, the data set has still been used to understand better and predict the performance of barrier components. The THM and THMC modeling activities related to the FEBEX-DP experiment were later embedded in other international initiatives, like the SKB EBS Task Force, but these have now ended. In FY24, SFWST researchers completed laboratory experiments to study coupled microbial-abiotic processes on bentonite samples exposed to 18 years of heating.

– The HotBENT Project is a full-scale high-temperature heater experiment conducted by several international organizations (including the U.S. DOE) to investigate the performance of bentonite buffers and near-field rock at maximum temperatures between 175°C and 200°C, which is higher than the 100°C maximum temperature generally assumed for clay-based repository materials. These higher temperatures may lead to potentially detrimental physicochemical changes in engineered and natural materials and may induce complex moisture transport processes. Construction of HotBENT was finalized in 2021, and the *in-situ* experiment officially started on September 9, 2021, when the heaters were turned on for the first time. After months of careful ramping up of heater power, all HotBENT heaters reached their final target temperatures of 175°C or 200°C in June 2022 and have been smoothly operating since. SFWST has been very active from the beginning of the HotBENT project and has made significant contributions: (1) Scoping calculations were conducted with simplified models to facilitate the design of the full-scale heater test; (2) High-temperature laboratory column tests and hydrothermal batch experiments have been carried out to provide information that cannot be measured in the field test; (3) Interpretive and predictive models have been developed and applied as part of the HotBENT Modeling Platform to deepen the understanding and improve modeling capabilities.

Other collaboratively conducted experiments at the GTS may also interest SFWST. This report briefly introduces some opportunities, including recently proposed new projects such as the

Advanced Corrosion Study Project or the Muon Tomography Proof-of-Principle Project. SFWST is following the progress of these projects and evaluating the benefit of joining additional GTS projects.

Collaboration with International Collaboration Projects Organized by SKB (Swedish Nuclear Fuel and Waste Management) (since 2015)

In the past, collaboration with SKB has primarily centered on the SKB Task Forces, but the planned dismantling of the Prototype Repository provides another valuable opportunity for collaboration.

- The SKB Task Forces are a forum for international collaboration related to conceptual and numerical modeling of performance-relevant processes in natural and engineered systems (currently 12 partners). One task force focuses on flow and radionuclide migration processes in naturally fractured crystalline rock (Groundwater Flow and Transport Task Force, Sweden (GWFTS) Task Force); another task force tackles the remaining challenges in predicting the coupled behavior of the engineered barrier system (EBS Task Force). While historically, both task forces have centered on experimental work conducted at the Äspö Hard Rock Laboratory (HRL) situated in crystalline rock, there have been more and more tasks in recent years that are generic or bring in experiments and data from other URLs. DOE joined both Task Forces in January 2014 and has been actively engaged. In the GWFTS Task Force, SFWST researchers are currently studying modeling approaches to predict flow channelized flow and reactive transport in fractured crystalline rock (Task 10). More activities are going on in the EBS Task Force: (1) The HotBENT Column Test conducted at LBNL was brought into the Task Force as supplying task description and experimental data and coordinating the coupled thermal-hydrological-mechanical (THM) modeling; (2) A SFWST scientist chairs Task 12 on modeling cement-bentonite interaction. LBNL and SNL have advanced in developing complex reactive transport models for this task.
- Another SKB-related opportunity is currently being discussed. SKB has initiated the dismantling of the inner section of their Prototype Repository Heater Test at the Äspö Hard Rock Laboratory (HRL), Sweden, which started operation in 2001. The full-scale test was the longest-operating multi-barrier repository experiment in the world. SKB has invited the international community to participate in this dismantling project. Scientists from SFWST met a few times with SKB in early 2023 to get clarity about the benefits and costs of joining the project as a research collaborator. SFWST and SKB have expressed their mutual interest, and SKB recently prepared a draft contract for DOE to consider. Currently, DOE is reviewing the draft contract.

The above collaborative initiatives foster active research projects, provide access to field and laboratory data, and/or may allow participation in field experiments in URLs. Complementing these activities, DOE or its national laboratories have engaged in collaboration opportunities provided by the Nuclear Energy Agency (NEA). Many of these NEA opportunities are less focused on active research collaboration rather than on the exchange of information or shared approaches, such as NEA's Integration Group for the Safety Case (IGSC), the Clay, Salt, and Crystalline Clubs, the Thermochemical Database Project, and the Information, Data and Knowledge Management (IDKM) Project. One exception: The NEA Horonobe International Project (HIP) was launched in 2023 to conduct international joint experiments and related analysis at the Horonobe URL in Japan, with eleven partner organizations from eight countries. The U.S. program is currently not engaged with HIP.

In FY24, SFWST also instituted a technical partnership with the EURAD-2 European Commission collaborative research program, which just launched a new round of repository R&D work for five years from 2024 through 2029. The goal is to allow SFWST scientists to collaborate in-kind with projects funded under EURAD-2 for cross-benefit between these two large research programs. Some of DOE's national laboratories were incorporated as Associated Partners into nine selected work package proposals for EURAD-2.

Bilateral Collaboration Opportunities (Section 4 of this report)

In addition to its extensive cooperation with multiple international organizations under the above-listed initiatives, the SFWST program has also explored direct bilateral opportunities for active research collaboration. It has selected additional R&D activities with the potential for substantial technical advances. The status of selected opportunities and activities is described below.

- Germany has emerged as one of the most important partners for active research collaboration. SFWST and German partners have a long history of collaborating on model benchmarking and data exchange for salt repositories in bedded and domal salt. The U.S.-German collaboration on salt currently comprises a range of topics, such as the performance of geotechnical barriers in salt formations and the coupled behavior of crushed rock salt as a drift backfill material. These topics are of particular importance for the design, operation, and evaluation of the long-term safety of underground repositories for disposal of high-level radioactive waste in salt. There are many other opportunities for joint research, as Germany, like the U.S., is now considering a broad range of host rocks and repository designs and has recently implemented a comprehensive repository siting program.
- DOE and the National Radioactive Waste Management Agency of France (Andra) have established a Memorandum of Understanding (MoU) regarding collaborative work in clay/shale disposal research at the LSMHM Underground Laboratory near Bure (also referred to as Bure URL), which is co-located with the French disposal site Cigeo in Meuse/Haute-Marne in the east of France. (LSMHM stands for Laboratoire de recherche Souterrain de Meuse/Haute-Marne, which translates to an underground laboratory in France's Meuse/Haute-Marne region.) Andra and U.S. researchers have been closely cooperating under the umbrella of the DECOVALEX Project. Andra is leading a modeling task in the current DECOVALEX-2027 Project, which focuses on gas migration in sand-bentonite mixtures using data from a field experiment at the Bure URL.
- Collaboration with a scientific deep drilling project in Sweden called COSC (Collisional Orogeny in the Scandinavian Caledonides) has provided a valuable opportunity for field testing of site characterization techniques in crystalline host rocks. Since 2017, SFWST scientists have conducted two major field campaigns using the deep borehole to develop and apply a multi-step monitoring workflow for the *in-situ* characterization of fractures, including their hydromechanical properties and stress states. This workflow was independently demonstrated in FY24 to characterize a fault zone at 1 km depth in the Bedretto URL in Switzerland (Hu et al., 2024). International collaboration on best practices and technologies for site selection and characterization is a longer-term goal in the SFWST Disposal Research R&D 5-Year Plan (Sassani et al., 2020; 2021; 2023).
- Other potential opportunities exist with several disposal programs, such as those from the Republic of Korea, Japan, Belgium, Finland, Czech Republic, and China. For example, the KURT in Korea, a generic underground research laboratory in a shallow tunnel in granite host rock, has been the subject of collaboration activities with SFWST in the past and would be open to more in the future. The Horonobe (sedimentary) and Mizunami (crystalline) URLs in Japan are accessible for SFWST participation under the JNEAP (Joint U.S.–Japan Nuclear Energy Action Plan) agreement. Belgium has an R&D program in geologic disposal and a long history of experimental work in its High Activity Disposal Experimental Site (HADES) underground research laboratories. Finland has already selected a site, submitted a license to operate, has almost finalized the construction of its disposal facility Onkalo near Olkiluoto, and is about to embark on a final step of getting ready for waste emplacement, the so-called Trial Run of Final Disposal. Construction of the repository has provided a wealth of relevant new data from the pilot hole and deposition

tunnel investigations, such as fracture frequencies, fracture trace maps, and groundwater inflows. The Czech Republic has an internationally oriented nuclear waste disposal program, and since 2017, has conducted *in-situ* testing in its Bukov Underground Research Facility in an existing mine in crystalline rock. The Czech radioactive waste management agency, SÚRAO, is expanding its experimental area for new experiments with the buildout of a second stage, referred to as Bukov URF II.

- China has launched an ambitious long-term URL R&D plan and started construction of its Beishan URL, which is also situated in crystalline host rock. As of May 2024, the shaft has been completed, the ramp has been advanced to 4,000 m using a tunnel boring machine, and excavation of the first working level has started. All these countries are open to collaboration with SFWST scientists.
- Bilateral collaboration opportunities may also be pursued to gain knowledge about international siting approaches and site characterization practices for geologic disposal via engagement with countries currently going through such efforts. Countries that come to mind are, for example, Germany, which is currently in the early stages of site selection considering the entire country and a broad range of host rocks, and Canada, which has narrowed its search from initially 22 volunteer areas to two sites, or Switzerland which has just down selected from three siting regions to one.

SFWST Research Activities Associated with International Collaboration (Section 6 of this report)

Starting in 2012, SFWST has established a balanced portfolio of international R&D activities in disposal science, addressing relevant R&D challenges in fields like engineered barrier integrity, near-field perturbation, radionuclide transport, integrated system behavior, performance assessment, site characterization, and monitoring approaches. These form a considerable portion of SFWST disposal research, and significant advances have been made over the past few years across different host rock types and engineered barrier research challenges. Figure ES-1 gives a visual overview of the significant international field experiments that SFWST researchers have participated in since 2012, either as active members of the experimental team or as researchers involved in the interpretative evaluation and model interpretation of the experimental data (see list of experiments in Table ES-1). The figure tries to graphically illustrate the balance and focus of SFWST's international program over the past years. There are a few notable observations:

- From the center outward, one can see that SFWST's research is well-balanced between an EBS focus, a near-field focus, and a far-field emphasis, utilizing field experiments conducted in multiple URLs in several countries.
- Several experiments address EBS behavior and near-field processes at the same time, which is no surprise because *in-situ* experiments in URL tunnels by design have near-field host rock impacts even if the main emphasis may be on the engineered barrier behavior.
- Many activities are related to field experiments in argillite and crystalline host rock, whereas less international work has been conducted for salt. This can be explained by the U.S. program having its salt URL in the bedded salts at the Waste Isolation Pilot Plant (WIPP) in New Mexico, so there is less need for international research outside the U.S.
- The topic of "Integrated System Behavior, Performance Assessment, and Site Characterization" features two full-scale demonstration experiments with SFWST participation, the FE Heater Test at the Mont Terri URL in Switzerland and the EBS Experiment at the Horonobe URL in Japan. In addition, SFWST is currently considering participation in the dismantling of SKB's Prototype Repository Heater Test, another demonstration experiment that has been running since 2001 at the Äspö Hard Rock Laboratory. SFWST also participates in the field-testing of new site characterization methods and workflows, such as at the COSC deep drilling site in Sweden, the

FEAR testing at the Bedretto URL in Switzerland, and the analysis of fracturing data from the Onkalo URL and repository site in Finland.

Overall, the focus on international collaboration has allowed deep engagement of U.S. researchers with the international waste management R&D community in terms of best practices, new science advances, state-of-the-art simulation tools, site characterization and monitoring approaches, lessons learned, etc. The joint R&D with international researchers, the worldwide sharing of knowledge and experience, and the direct access to relevant data/experiments from various URLs and host rocks have helped SFWST researchers significantly improve their understanding of the technical basis for disposal in different host rock environments. Comparison with experimental data has contributed to testing and validating predictive computational models for evaluating disposal system performance in various generic disposal system concepts. Comparison of model results with other international modeling groups, using their simulation tools and conceptual understanding, have enhanced our confidence in the robustness of predictive models used for performance assessment. The possibility of linking model differences to conceptual model setup provides valuable guidance into "best" modeling choices and understanding the effect of conceptual model selection on prediction uncertainty. Such advances in making long-term predictions of complex coupled THMC and flow and transport processes contribute directly to improving post-closure PA models. Access to international field testing also provides an opportunity to develop, test, and demonstrate new methods and workflows for site characterization and monitoring of deep geological disposal. International collaboration finally provides opportunities for training/educating junior staff well suited to move the U.S. disposal research program forward into the next decades. Selected highlights of recent SFWST research advances related to international collaboration are given below:

Coupled Processes and Alterations in Bentonite-Based Engineered Barrier Systems

Collaborations with the international FEBEX-DP, HotBENT, and Horonobe EBS projects involve large-scale experimental and modeling studies to understand temperature-dependent perturbations and alterations in engineered barrier materials. These activities have provided valuable insights into how these perturbations and alterations may affect repository performance.

- Participation in the large-scale FEBEX *in-situ* heater test and its comprehensive dismantling effort after 18 years of operation has significantly enhanced the understanding of the thermal alteration of EBS materials. The post-mortem FEBEX-DP bentonite samples continue to provide a basis for evaluating potential EBS property changes. The results of laboratory-scale experiments investigating coupled microbial-abiotic processes in altered and unaltered bentonite samples indicate considerable metabolic potential within the microbial communities even after long-term exposure to heat. This is important because microorganisms that survive in a nuclear waste repository can later become active as gas is introduced or produced in the system, water is introduced through cracks in the containment or other environmental changes.
- Since reaching its final target temperature of 175°C or 200°C in June of 2022, the HotBENT field test has provided data on bentonite behavior at strongly elevated temperatures, which are now used for interpretative modeling. LBNL has developed a 3D thermal-hydrological (TH) model, which can match the trends observed in the thermal and hydrodynamic behavior of the EBS. However, the current model underpredicts the temperature of the bentonite near the heaters. LBNL plans to extend the 3D TH model to a 3D THM and possibly the THMC model, improving the model predictions, especially regarding the buffer's hydration behavior.
- In support of the HotBENT field test, SFWST researchers conducted a series of high-temperature laboratory column tests using innovative geophysical imaging techniques. In FY24, the team studied and simulated results from the HotBENT-Lab #2 column test, which used granulated Wyoming bentonite and lasted 16 months. The laboratory experiment provides a unique data set

of the spatio-temporal change of bentonite properties affected by hydration, heating, and swelling.

- TH simulations were conducted with the PFLOTRAN simulator to understand engineered barrier alterations associated with the JAEA EBS design concept. This work was done under the DECOVALEX-2023 model comparison project, where Task D comprises the full-scale EBS Experiment at the Horonobe URL in Japan. It was shown that a reduced order 2D model, instead of a full 3D model, can well represent the general temperature trends. Improvement of the 2D PFLOTRAN model is needed to simulate fluid flow affected by mechanical processes, such as bentonite swelling and related couplings with porous media flow.

Alterations at the Interface Between EBS and Host Rock Materials

Several international collaboration studies made significant progress in evaluating interfacial reactions between EBS components and host rock materials. Materials alterations near these interfaces can affect repository performance in multiple ways, for example, by changing the flow and transport properties for radionuclides to migrate from the engineered into the natural barrier systems. Interfacial reactions are most prominent early in a repository's lifetime when EBS materials such as bentonite, metal containers, and cementitious materials have just been emplaced and when TH perturbations remain strong.

- Hydrothermal laboratory experiments were conducted to better understand interfacial material alterations in conditions relevant to the EBS experiment at the Horonobe URL in Japan and the HotBENT experiment at the Grimsel Test Site in Switzerland. The experimental findings suggest that the tested bentonites may only experience slight alteration during the initial thermal pulse in a repository setting. The mineralogical and geochemical changes observed in both experimental settings can be applied to develop conceptual and numerical models for assessing long-term material stability in a high-temperature repository.
- Laboratory experiments were conducted to study bentonite erosion, coagulation/flocculation, and fracture clogging behavior under controlled conditions. Results demonstrated the need to develop a new experimental setup to study erosion and coagulation from a single experimental system because a combination of erosion and coagulation will ultimately govern colloid transport. Future experiments will be conducted using unaltered versus hydrothermally aged/altered bentonite to understand the parameters that significantly impact bentonite erosion and coagulation in geochemical conditions relevant to nuclear waste repositories. This work is loosely connected to international collaboration efforts conducted in the CFM and FEBEX projects.
- Reactive transport simulations were performed to interpret interfacial reactions and their impact across aged bentonite, concrete/cement, and clay rock interfaces. These activities were aligned with (1) the international CI-D experiment, which probes diffusive transport across materials placed in a borehole at the Mont Terri URL about 14 years ago, and (2) the reactive-transport modeling of cement-bentonite interaction as part of the SKB EBS Task Force Task 12 benchmarking activities:
    - Simulations of the CI-D cement-clay interaction test at Mont Terri using the CrunchClay software, which considers electrostatic effects in the electrical double layer (EDL) models, demonstrated the need to extend the duration of modeling and use a more comprehensive reaction network to predict long-term cement and cement-clay interactions.
    - The Task 12 benchmarking of geochemical changes due to cement-bentonite interaction showed substantial changes in pore solution chemistry, particularly at early times. This can lead to considerable alteration of highly soluble minerals, significantly changing the porosity and permeability near the interface and possibly impacting the long-term migration of

radionuclides through a cement-bentonite EBS. However, the simulations also demonstrated that areas with significant mineral alteration are limited to a few cm near the interface. Future work should be devoted to evaluating the safety implications of these complex interfacial alterations.

THM Processes in Heated Argillaceous Rock

Through access to several *in-situ* heater experiments, SFWST scientists made significant scientific advances in understanding and predicting the THM perturbations occurring in argillaceous host rock after the emplacement of heat-emanating radioactive waste.

- The full-scale FE heater test at Mont Terri, now in its 10th year of heating, continues to provide valuable THM data at relevant spatial and temporal scales. Under the umbrella of Task C of the DECOVALEX-2023 initiative, SFWST researchers and several international partners worked on interpretative and comparative THM simulations for model validation. Based on a comprehensive sensitivity study, the teams achieved an excellent overall match with the measured pore pressure changes in the host rock when considering reduced near-field permeability and increased fluid storage. After completing the work with DECOVALEX-2023, LBNL will resume regular Mont Terri project simulations of the 10-year field data at the FE Experiment. The work for the Mont Terri project will focus on the interaction of the host rock with the bentonite buffer and the stress in the bentonite buffer.
- The ability to simulate processes and mechanisms of thermal fracture initiation was tested in Task A of the DECOVALEX-2023 initiative. Modeling of the CRQ *in-situ* heating experiment at the Bure URL showed that different THM modeling approaches could reproduce spatial-temporal fracture initiation in the COx clay rock. In contrast, attempts to reproduce fracture aperture or fracture propagation were less accurate and require more work in the future.

Gas Transport in Bentonite and Clay-Based Host Rock

Gas generation from canister corrosion and other processes can impact the performance of a geological disposal facility in several ways. For example, the gas-water interfaces are essential for transporting radionuclides and microorganisms due to channelized flow and preferential sorption. In contrast, trapped gas bubbles can cause accumulation or immobilization of radionuclides. Local pressure build-up due to gas production and accumulation can trigger mechanical responses such as deformation or fracturing in low-permeability materials like bentonite and clays. Significant progress was made in understanding the short- and long-term processes involved in generating and migrating repository gases.

- Under the umbrella of the DECOVALEX-2023 initiative, SFWST scientists and their international partners tested their predictive capabilities for gas migration against data from the full-scale LASGIT experiment conducted at the Äspö Hard Rock Laboratory in Sweden. LBNL scientists were able to show that a hydro-mechanical (HM) modeling approach that was initially developed to simulate small-scale gas injection laboratory experiments could be extended to match the LASGIT field observations.
- A new conceptual model was developed to best capture the complex phenomenological behavior of gas flow through bentonite. The latest model can represent observed gas migration patterns such as rapid breakthrough, aperiodic/chaotic gas flux, fast percolation, and low gas saturation. Due to fractal scale invariance, this may provide a new perspective for upscaling from small-scale laboratory observations to a field scale. Based on the linear stability analysis theory, it was shown that gas channeling can emerge from the morphological instability of the interface between the injected gas and the compacted bentonite due to local stress concentration, pore dilation, and hydrologic gradient variation.

Coupled Processes, Fluid Flow and Transport in Fractured Crystalline Rock

Because crystalline formations are often fractured, repository performance assessment studies require an understanding of (1) the impact of stress changes and other perturbations on fracture flow and transport properties and (2) the ability to simulate large-scale transport patterns of radionuclides migrating in fracture networks from the repository to the biosphere. Two international collaboration activities have made significant progress in addressing these challenges.

- Task G of the DECOVALEX-2023 initiative involved thermo-mechanical (TM) and HM modeling of single fracture mechanics exposed to complex stress states. A comparison of simulations conducted by national lab scientists with other international modeling teams showed that complex TM and HM experiment results could be understood and reproduced numerically with sufficient accuracy to represent main process characteristics. Micro-scale TM simulations of thermal shearing laboratory experiments identified the fundamental properties impacting shearing behavior in flat and rough fracture surfaces. Modeling results of HM processes evaluated the effects of axisymmetric and triaxial loadings on the surface normal stress, surface displacement, and surface strain. It used these results to estimate hydraulic aperture and fracture permeability changes. The collaborative model comparison conducted in Task G will improve the reliability and predictability of models for fracture flow and transport in crystalline rock.
- Numerical modeling conducted under the umbrella of the SKB GWFTS Task Force focused on characterizing the impact of finite matrix block size on particle transport through fracture networks. It was shown that the travel time distributions through fracture networks with finite blocks are similar to those with infinite blocks when the fracture spacing is sufficiently large, matrix diffusion is relatively weak, or transport is considered at an early control plane distance. These results provide a first step toward developing a metric to assess when finite block size effects are expected to significantly influence transport, which could be critical for repository assessment.
- A new mesh generation methodology for 3D discrete fracture networks and the adjacent rock matrix (nMAPS) was developed, robustly tested, and integrated into Los Alamos National Laboratory (LANL)'s powerful gridding toolkit. This new meshing capability will better represent geological features and repository structures in GDSA PA simulations.

Coupled Processes in Salt

A broad portfolio of international collaboration has resulted in significant advances in understanding complex mechanical, hydrological, thermal, and chemical processes in salt.

- Collaborative research with German institutions included (1) assessing geotechnical barriers in salt in the collaborative project RANGERS and (2) improving THM modeling for crushed salt (used as backfill for repository tunnels) in the joint KOMPASS and MEASURES projects.
  - The RANGERS Project completed a comprehensive compilation of existing knowledge and experience about geotechnical barriers in a salt repository. A key outcome of the work is a set of recommendations for designing and verifying geotechnical barriers based on the state of the art in science and technology.
  - The KOMPASS Project completed experimental investigations of microstructural effects on compaction methods and conducted a comparative THM model evaluation. Each modeling partner calibrated their model against laboratory tests performed on KOMPASS reference material, developed model improvements as necessary, and used the resulting calibrated model(s) to simulate the closure of a drift backfilled with crushed salt. Sandia began developing a new crushed salt constitutive model as part of the MEASURES proposal.

- International collaboration within the framework of Task E of the international DECOVALEX-2023 initiative allowed SFWST scientists to benefit from the engagement of international partners in the analysis and modeling of brine migration in heated salt. THM modeling conducted by the joint team of LBNL, Sandia National Laboratory (SNL), and LANL researchers captured the main characteristics observed in the BATS heater experiment at WIPP, including modeling of the cooling-induced increase in brine inflow after heater turn-off and the evolution of damage in rock salt during heating and cooling. This work helped improve understanding of the complex processes expected to occur in the Excavation Damaged Zone (EDZ) of a salt repository for disposal of heat-generating radioactive waste and supports building the long-term repository safety case for radioactive waste disposal in salt. Under the leadership of SNL scientists, the collaborative salt modeling of recent BATS experiments continues in the current DECOVALEX-2027 phase.
- Under the NEA Salt Club umbrella, SFWST and international colleagues continued to develop a comprehensive Features, Events, and Processes (FEPs) database for salt host rock. They extended these efforts towards a generalized approach to scenario development for a high-level waste repository at a generic salt site.

Hydromechanical Behavior of Faults and Fractures in Response to Repository-Induced Perturbation in Argillite Host Rock

Via field-based and simulation-based research, SFWST scientists made important advances in understanding whether and for how long faults and fractures in low-permeability host rock such as clay rock can be potential radionuclide migration pathways upon activation from repository-induced effects.

- SFWST scientists advanced the data and modeling analysis of the Mont Terri fault reactivation experiments to explore the ability of reactivated faults to self-seal over time. Integrating *in-situ* experiments and modeling revealed several key mechanisms contributing to the observed self-sealing phenomena following the activation of a shale fault. Time estimates for the return of a fault to its initial small transmissivity project are a minimum of 50 years.
- Efficient machine learning (ML) approaches were developed for predicting fault reactivation processes, utilizing data from the 2020 fault reactivation conducted at the Mont Terri URL. LBNL researchers tested a specific protocol for training the ML model, which ensures that the model can accurately represent the complex fault response both qualitatively and quantitatively during and after injection.

Characterization of Fractured Crystalline Rock

A key concern related to geologic disposal in fractured crystalline rock is the presence of potentially conductive fractures that could result in the transport of radionuclides. There is a need for improved hydrological, geomechanical, and geochemical techniques for the *in-situ* characterization of fractures including their hydromechanical properties and stress states.

- In cooperation with Sweden's COSC deep drilling project, the deep borehole COSC-1 was used as a testbed for advanced site characterization of fractured crystalline rock. SFWST scientists developed and tested a new workflow using novel downhole probes to identify flowing fractures, evaluate their HM properties, and estimate the state of stress in the subsurface.
- Analysis of the COSC-1 data demonstrated that adding borehole displacement measurements to a standard hydraulic fracturing test allows for an accurate estimation of fracture HM properties (stiffness, hydraulic aperture), intact rock bulk and shear moduli, and local state of stress.
- To demonstrate that the Step-Rate Injection Method for Fracture *In-situ* Properties (SIMFIP) deep borehole characterization workflow is mature, SFWST scientists recently deployed their method

to characterize a crystalline host rock in the Bedretto URL (Switzerland), which provides access to a fault zone at a 1 km depth. Compared to the COSC-1 experiments in Sweden, the Bedretto tests highlighted that a fault zone may create significantly greater stress perturbations than single fractures. More experimental and interpretative work related to the Bedretto URL will be conducted in FY25.

Performance Assessment and Radionuclide Transport Modeling

Recognizing the importance of building confidence in the models, methods, and software used for PA of deep geologic repositories, SFWST researchers have increased their international collaboration in this area.

- In Task F of the DECOVALEX-2023 initiative, confidence in performance assessment models and methods was enhanced by comparing PA modeling results from ten international disposal programs applied to the same reference cases, one involving a repository in a fractured crystalline host rock and another featuring a repository in a bedded salt formation. The comparison of performance assessment approaches continues in the current DECOVALEX-2027 phase, with an enhanced focus on sensitivity analysis and uncertainty quantification.
  - The crystalline reference case highlighted the importance of explicitly including drifts, buffers, and backfill in the simulations. For models with a comparable repository geometry and inventory evolution, the primary source of model uncertainty was the choices of how to represent the fracture network and simulate the transport of two tracers. Overall, the modeling results showed considerable discrepancies and demonstrated the importance of examining multiple modeling approaches in performance assessment.
  - Despite deploying different modeling strategies, all PA models for the salt reference case in Task F of DECOVALEX-2023 showed that the engineered barriers are effective for containing the radionuclides in the repository and that only a small amount of the disposed of radionuclides will migrate beyond the repository seal over 100,000 years. All models also indicate that salt compaction and radionuclide diffusion are critical physical processes in the simplified repository system.
- SFWST scientists play a crucial role in disseminating sorption data and acting as good data stewards by updating their improved database in a consistent format and assessing the quality of the newly assimilated data in an organized fashion. To this end, all data and workflows are open-access and made available on a Lawrence Livermore National Laboratory (LLNL) website (https://seaborg.llnl.gov/resources/geochemical-databases-modeling-codes).
- The continued international collaboration of LLNL researchers within the NEA Thermochemical Database Project led to significant improvements in thermodynamic and thermochemical databases and models for radionuclide transport simulations. The goal is to produce interoperable open-source databases that harness modern data science workflows and algorithms.

Next Generation Workforce Development

Investing in the next generation of diverse, talented nuclear waste scientists and leaders is vital to fulfilling DOE NE’s mission of developing solutions for the long-term geologic disposal of radioactive waste. In FY22, the SFWST program established a three-year Next Generation Workforce Development Pilot Program to attract, train, and advance a talented and diverse future workforce. LBNL and SNL started the Program in FY22, and LANL was brought into the program in FY23. International collaboration is essential in this context. To help recruit and train a broad talent pool, the workforce development program has provided interesting learning/research challenges and attractive work-abroad opportunities in conjunction with SFWST’s multiple international collaboration partners. While FY24 marks the final year of the 3-year pilot, the program has been a great success, and SFWST envisions the program's continuation in the foreseeable future.

- Stimulating Student Interest in Nuclear Waste Research: Between FY22 and FY24, the Next Generation Workforce Development Pilot Program inspired many students to become interested in nuclear waste disposal science through lab-university-organized lectures and seminars. National lab scientists held in-person and hybrid classes at the University of New Mexico and the University of Puerto Rico ~ Mayaguez. A webinar series named "Next Generation Workforce Development for Spent Fuel and Waste Science and Technology" was co-organized by MIT, Texas A&M, SNL, and LBNL.
- Creating the Pipeline: Over the past three years, the summer internship program has trained a large, diverse student group of 29 interns at LBNL, SNL, and LANL. This created a pipeline: Many of the summer interns returned to their hosting national lab (or other opportunities) after their initial summer program ended, either for another summer program or in some cases as year-round interns. At LBNL, three summer interns were hired as postdoctoral researchers.
- Advancing the Pipeline: LBNL and SNL each hired a dedicated "next generation" postdoc for a three-year research project with international collaboration, which allowed them to make remarkable research contributions. For example, LBNL's dedicated postdoc has worked on THM modeling for the international HotBENT Project and, to connect her with the international community better, participated in a 2023 summer training program at the Grimsel Test Site. SNL's dedicated postdoc works in GDSA Repository Safety Assessment (RSA), incorporating geology into uncertainty quantification and sensitivity analysis (UQ/SA).

Outlook for International Collaboration (Sections 5 and 7)

In the future, international collaboration will continue to be an essential cross-cutting campaign activity within the SFWST campaign. SFWST's recent strategic 5-year plan emphasizes international collaboration as a central element of the campaign's disposal research portfolio. It defines a comprehensive list of near-term to mid-term goals for continued collaboration activities (Sassani et al., 2023). SFWST considers elevating international collaboration in disposal research to a new level of emphasis and recognition, by establishing a Center for International Collaboration in Disposal Research at LBNL.

The international research portfolio has evolved and will grow as research priorities change and new collaboration opportunities emerge. The campaign routinely reviews, assesses, and develops such opportunities in close integration with international partners, evaluates the technical merit and alignment with the SFWST objectives, and revises the portfolio of international R&D activities as appropriate. Given its importance within the overall portfolio of disposal research activities, any such planning and prioritization is done in tight integration with all other disposal research areas, e.g., the host-rock-specific research portfolios, the EBS research portfolio, and the performance assessment research portfolio. This report identifies several additional opportunities for international collaboration that the campaign may consider going forward, including new international field experiments and opportunities related to international siting approaches and site characterization practices.

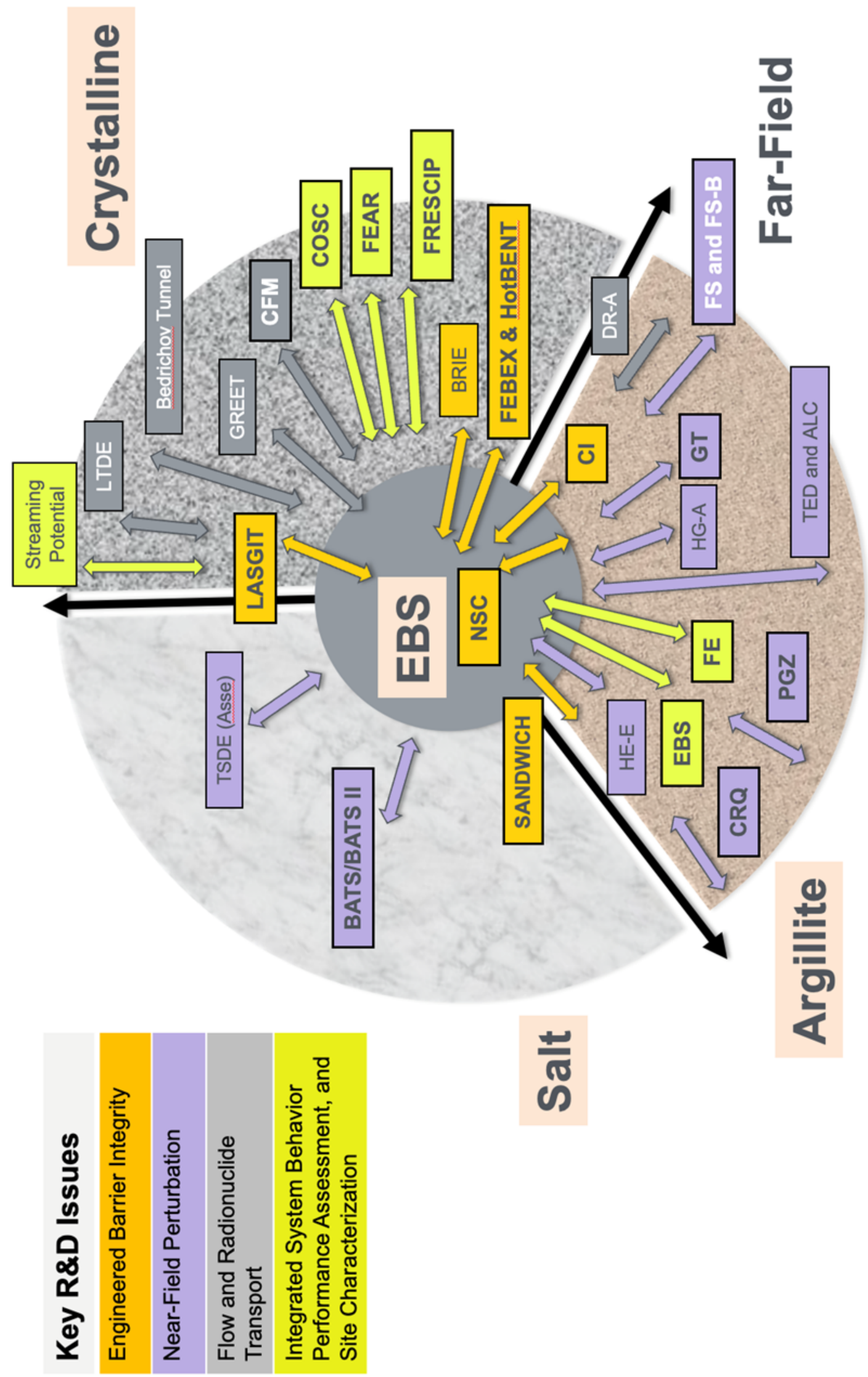

Figure ES-1. A high-level overview of the major field international URL experiments conducted in various countries that SFWST researchers have participated in since 2012. Experiments in bold denote currently active collaborations. See Table ES-1 for more information on each experiment. Status: FY24.

Table ES-1. A high-level overview of the major international URL experiments conducted in various countries that SFWST researchers have participated in since 2012. Experiments in bold denote currently active collaborations. Status: FY24.

Key Topics	International Experiment	URL	Main R&D Focus
Engineered Barrier Integrity	Bentonite-Rock Interaction Experiment (BRIE)	Äspö HRL, Sweden	Understand the impact of flowing fractures in crystalline rock on bentonite saturation, integrity and erosion
	Full-Scale Engineered Barrier Experiment - Dismantling Project (FEBEX-DP)	Grimsel Test Site, Switzerland	Dismantling and sampling of long-term test evaluating the long-term integrity and performance of heated bentonite
	Large-scale Gas Injection Test (LASGIT)	**Äspö HRL, Sweden**	***In situ* monitoring of gas migration processes in bentonite buffer**
	HotBENT Experiment	**Grimsel Test Site, Switzerland**	**Complex THMC behavior of EBS materials up to 200 degrees C at the canister/bentonite interface**
	SANDWICH Experiment	**Mont Terri, Switzerland**	**Testing the HM behavior of a novel shaft-sealing system with alternating sealing layers**
	NSC Bentonite-Sand Sealing Experiment	**Bure, France**	**Evaluating the seal performance of a gas permeable bentonite-sand mixture at full tunnel scale**
Near-Field Perturbation	Heater Experiment E (HE-E)	Mont Terri, Switzerland	Bentonite/rock interaction to evaluate sealing and clay barrier performance at elevated temperature
	Thermal Experiment (TED) Full-scale Emplacement Test (ALC)	Bure, France	Upscaling THM simulations from lab tests to repository scale
	Gas Path Though Host Rock Experiment (HG-A)	Mont Terri, Switzerland	Evaluation of flow paths through the near-field damage zone and specifically along seals
	Thermal Simulation for Drift Emplacement (TSDE)	Asse Mine, Germany	Model benchmarking studies for thermal-hydrological-mechanical behavior salt heater test
	CRQ Thermal Fracturing Experiment	**Bure, France**	**Testing the behavior of argillite host rock to a thermal fracturing stress regime**
	PGZ Gas Fracturing Test	**Bure, France**	**Testing the behavior of argillite host rock upon high-pressure gas injection**
	Fault Slip Experiments FS and FS-B	**Mont Terri Switzerland**	**Fault reactivation and permeability generation due to repository-induced effects in a clay rock**
	Brine Availability Test in Salt (BATS)	**WIPP, USA**	**Monitoring brine distribution, inflow, and chemistry from heated salt using geophysical methods and direct liquid & gas sampling**
	GT Experiment	**Mont Terri, Switzerland**	**HM testing of argillaceous host rock responding to gas injection and migration**
	STIMTEC Experiment	**Reiche Zeche, Germany**	**Fluid injection into crystalline rock mass and measurements of microseismicity**
Flow and Radionuclide Transport	Bedrichov Tunnel Experiment	Bedrichov, Czech Republic	Interpretation of water inflow patterns and tracer transport behavior in fractured granite
	GREET (Groundwater Recovery Experiment)	Mizunami, Japan	Evaluation of early resaturation behavior in crystalline rock looking at flow behavior and chemical-biological interactions upon resaturation
	Long-Term Sorption Diffusion Experiment (LTDE)	Äspö HRL, Sweden	Monitoring the diffusion behavior in fractured crystalline rock
	DR-A Experiment (Diffusion Retention and Perturbation Test)	Mont Terri, Switzerland	Ion diffusion through compacted clay where electro-chemical charges affect transport behavior
	Colloid-Facilitated Radionuclide Migration Test (CFM)	**Grimsel Test Site, Switzerland**	**RN transport of bentonite colloids compared in a shear zone in fractured granite**
Integrated System Behavior, Performance Assessment, and Site Characterization	Streaming Potential Test	KURT, Korea	Testing a new site characterization technique to measure deep groundwater flow
	Engineered Barrier System (EBS) Experiment	**Horonobe, Japan**	**Full-scale studies of the thermo-hydro-mechanical-chemical (THMC) behavior of the EBS**
	Full-scale Emplacement Experiment (FE)	**Mont Terri, Switzerland**	**Full-scale demonstration experiment, one of the largest and longest-duration heater tests**
	COSC Experiment	**Deep Drilling Project, Sweden**	**Testing new methods and workflows for borehole-based HM fracture characterization**
	FEAR Experiment	**Bedretto, Switzerland**	**Fault characterization and reactivation in deep crystalline rock**
	FRESCIP	**Onkalo URL, Finland**	**Fractured rock characterization and inflow prediction using data from repository construction**

ACKNOWLEDGMENTS

This work was supported by the Office of Spent Fuel and Waste Science and Technology, Office of Nuclear Energy, of the U.S. Department of Energy under Contract Number DE-AC02-05CH11231 with Lawrence Berkeley National Laboratory. Support of the work by Lizz Mahoney (LBNL) for formatting and proofing of this document is very much appreciated. We also appreciate the helpful discussions and insights from Prasad Nair (DOE NE-81), Tim Gunter (DOE NE-81), Bill Boyle (DOE NE-81), David Sassani and Emily Stein (SNL).

The authors are thankful to all contributors to the FY24 milestone reports of the SFWST program which have been used as input in this overview of international activities. A list of the SFWST reports and their authors is given in Section 8.1.

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ACRONYMS

1D	One-Dimensional
2D	Two-Dimensional
3D	Three-Dimensional
ACT	Advanced Corrosion Test
Andra	National Radioactive Waste Management Agency, France
BASE	Federal Office for the Safety of Nuclear Waste Management, Germany
BATS	Brine Availability in Salt Experiment, WIPP, New Mexico
BCV	Czech Bentonite (BCV) from Cerny Vrch deposit (north western region of the Czech Republic)
BGE	Federal Company for Radioactive Waste Disposal, Germany
BGR	Federal Institute for Geosciences & Natural Resources, Germany
BGS	British Geological Survey
BMT	Benchmark Test
BMWi	Ministry for Economy and Labor, Germany
BRIE	Bentonite Rock Interaction Experiment, Äspö HRL, Sweden
BRIUG	Beijing Research Institute of Uranium Geology
BTC	Breakthrough Curve
CASSM	Continuous Active-Source Seismic Monitoring
CFM	Colloid Formation and Migration Project, Grimsel Test Site, Switzerland
CI	Cement Interaction Test, Mont Terri, Switzerland
CI-D	Cement Clay Interaction Experiment, Mont Terri, Switzerland
CIEMAT	Centro Investigaciones Energéticas Medioambientales y Tecnológicas, Madrid, Spain
CNL	Constant Normal Load
CNM	Channel Network Model
CNS	Constant Normal Stiffness
CNSC	Canadian Nuclear Safety Commission
COSC	Collision Orogeny in the Scandinavian Caledonides
COx	Callovo-Oxfordian Claystone
CRIEPI	Central Research Institute of Electric Power Industry, Japan
CRQ	Representative THM Behavior of a High-Level Waste (HLW) Cell
CT	Computed Tomography
CU	Consolidated Undrained
DAS	Distributed Acoustic Sensing
DECOVALEX	DEvelopment of COupled Models and their VALidation Against EXperiments
DFN	Discrete Fracture Network

DITUSC	Development and Improvement of Thermodynamic Understanding for Use in Nuclear Waste Disposal Safety Case
DOE	Department of Energy, USA
DPC	Dual Purpose Canister
DR-A	Diffusion, Retention, and Perturbation Experiment, Mont Terri, Switzerland
DR-C	Thermal Diffusion Test, Mont Terri, Switzerland
DSS	Distributed Brillouin Strain Sensing
DW	Deionized Water
EB	Engineered Barrier
EBS	Engineered Barrier System
ECPM	Equivalent Continuous Porous Medium
EDL	Electrical Double Layer
EDZ	Excavation Damage Zone (or Excavation Disturbed Zone)
ENRESA	National Radioactive Waste Corporation, Spain
ENSI	Swiss Federal Nuclear Safety Inspectorate, Switzerland
EPA	U.S. Environmental Protection Agency
ERT	Electrical Resistivity Tomography
ETH	Swiss Federal Institute of Technology, Zurich
EURAD	European Joint Program on Radioactive Waste Management
FANC	Federal Agency for Nuclear Control, Belgium
FE	Full-scale Emplacement Experiment, Mont Terri, Switzerland
FEAR	Fault Activation and Earthquake Rupture, Bedretto URL, Switzerland
FEBEX	Full-Scale Engineered Barrier Experiment, Grimsel Test Site, Switzerland
FEBEX-DP	FEBEX Dismantling Project
FEPs	Features, Events, and Processes
FFEC	Flowing Fluid Electrical Conductivity
FORGE	Fate of Repository Gases
FS	Faults Slip Hydro-Mechanical Characterization Experiment, Mont Terri, Switzerland
GAST	Gas Permeable Seal Test, Grimsel Test Site, Switzerland
GDSA	Geologic Disposal Safety Assessment
GRS	Gesellschaft für Anlagen- und Reaktorsicherheit, Germany
GT	Gas Transport Experiment, Mont Terri, Switzerland
GTS	Grimsel Test Site, Switzerland
GW	Groundwater
GWFTS	Groundwater Flow and Transport Task Force, Sweden
HADES	High Activity Disposal Experimental Site, Mol, Belgium
HE-E	Heater Experiment in Micro-tunnel, Mont Terri, Switzerland
HG-A	Gas Path through Host Rock and Seals Experiment, Mont Terri, Switzerland

HIP	Horonobe International Project, Horonobe URL, Japan
HM	Hydro-Mechanical
HMC	Hydro-Mechanical-Chemical
HRL	Hard Rock Laboratory
IAEA	International Atomic Energy Agency
i-BET	In-Situ Bentonite Erosion Test, Grimsel Test Site, Switzerland
IDKM	Information, Data, and Knowledge Management
IfG	Institute für Gebirgsmechanik
IGSC	Integration Group for the Safety Case
IRSN	Institut de Radioprotection et de Sûreté Nucléaire, France
ISC	Importance to Safety Case
ISCO	International Steering Committee
JAEA	Japan Atomic Energy Agency, Japan
JCS	Joint Compressive Strength
JFCS	Joint Fuel Cycle Studies
JNEAP	U.S.–Japan Nuclear Energy Action Plan
JRC	Joint Roughness Coefficients
KAERI	Korea Atomic Energy Research Institute, Republic of Korea
KICT	Korea Institute of Civil Engineering and Building Technology, Republic of Korea
KIGAM	Korea Institute of Geoscience and Mineral Resources, Republic of Korea
KIT	Karlsruhe Institute of Technology, Karlsruhe, Germany
KORAD	Korea Radioactive Waste Agency, Republic of Korea
KURT	KAERI Underground Research Tunnel, Republic of Korea
LANL	Los Alamos National Laboratory, USA
LASGIT	Large-Scale Gas Injection Test, Äspö HRL, Sweden
LBNL	Lawrence Berkeley National Laboratory, USA
LIT	Long-Term In-Situ Test, Grimsel Test Site, Switzerland
LLNL	Lawrence Livermore National Laboratory, USA
LSMHM	Laboratoire de recherche Souterrain de Meuse/Haute-Marne
LSTM	Long Short-Term Memory
LTD	Long-Term Diffusion, Grimsel Test Site, Switzerland
LTDE	Long-Term Diffusion Sorption Experiment, Äspö HRL, Sweden
M	Mechanical
MA	Microbial Activity Test, Mont Terri, Switzerland
MACOTE	Materials Corrosion Test, Grimsel Test Site, Switzerland
MISP	Ministry of Science, ICT, and Future Planning, Republic of Korea
ML	Machine Learning
MoU	Memorandum of Understanding

MWCF	Major Water Conducting Feature
Nagra	Swiss Waste Management Organization
NBS	Natural Barrier System
NE	Nuclear Energy
NEA	Nuclear Energy Agency
NMM	Numerical Manifold Method
NSC	Noyau de Scelement Experiment (translates to Sealing Core)
NUMO	Nuclear Waste Management Organization of Japan
NWMO	Nuclear Waste Management Organization, Canada
NWS	Nuclear Waste Services, United Kingdom
OBAYASHI	Construction, Engineering and Management Company, Japan
OPA	Opalinus Clay
OPC	Ordinary Portland Cement/Concrete
PA	Performance Assessment
PNNL	Pacific Northwest National Laboratory, USA
POSIVA	Nuclear Waste Management Organization, Finland
PSI	Paul Scherrer Institute, Switzerland
QOI	Quantities of Interest
R&D	Research and Development
RE	Research Entity
REPRO	Rock Matrix Retention Properties, Onkalo URL, Finland
RH	Relative Humidity
ROK	Republic of Korea
RSA	Repository Safety Assessment
RWM	Radioactive Waste Management Limited, UK
RWMC	Radioactive Waste Management Committee
SA	Sensitivity Analysis
SAL	State of the Art Level
SCK/CEN	Belgian Nuclear Research Centre, Belgium
SET	Borehole Sealing Test, Grimsel Test Site, Switzerland
SFMWG	Spent Fuel Management Working Group
SFWST	Spent Fuel and Waste Science and Technology
SIMFIP	Step-Rate Injection Method for Fracture In-Situ Properties
SKB	Swedish Nuclear Fuel and Waste Management, Sweden
SNF	Spent Nuclear Fuel
SNL	Sandia National Laboratories, USA
SP	Streaming Potential
SSM	Swedish Radiation Safety Authority
SURAO	Radioactive Waste Repository Authority, Czech Republic

SW-A	Sandwich Experiment, Mont Terri, Switzerland
swisstopo	Federal Office of Topography, Switzerland
SWRCs	Soil Water Retention Curves
TC	Test Case
TDB	Thermochemical Database Project
TDE	Through Diffusion Experiment, Onkalo URL, Finland
TDR	Time Domain Reflectometry
TH	Thermal-Hydrological
THC	Thermal-Hydrological-Chemical
THM	Thermal-Hydrological-Mechanical
THMC	Thermal-Hydrological-Mechanical-Chemical
TM	Thermo-Mechanical
TSDE	Thermal Simulation for Drift Experiment, Asse Mine, Germany
TSO	Technical Support Organizations
TUC	Clausthal University of Technology, Germany
UFD	Used Fuel Disposition
UFZ	Umweltforschungszentrum Leipzig-Halle, Germany
UPC	Polytechnic University of Catalonia, Barcelona, Spain
UQ	Uncertainty Quantification
URL	Underground Research Laboratory
WIPP	Waste Isolation Pilot Plant, New Mexico, USA
WMO	Waste Management Organizations
XCT	X-Ray Computed Tomography
XRD	X-Ray Diffraction
XRF	X-Ray Fluorescence

1 INTRODUCTION

Since 2012, in an effort coordinated by LBNL, the Office of Spent Fuel and Waste Science and Technology (SFWST) within the U.S. Department of Energy (DOE) has advanced active collaboration with several international geologic disposal programs in Europe, North America, and Asia. Such collaboration has allowed the SFWST Campaign to benefit from a deep knowledge base regarding alternative repository environments developed over decades and has provided a framework for active peer-to-peer research participation in international groups, which conduct, analyze, and model performance-relevant processes. Via international collaboration, the SFWST Campaign also benefits from substantial international investments in research facilities (such as underground research laboratory testing and modeling) and achieves cost savings via joint funding of expensive field experiments. To date, SFWST's International Disposal R&D Program has established formal collaboration agreements with several international initiatives and various international partners. National lab scientists associated with SFWST have participated in a balanced portfolio of international R&D activities in disposal science, addressing relevant R&D challenges in fields like near-field perturbation, engineered barrier integrity, radionuclide transport, and integrated system behavior, performance assessment, and repository siting. These form a considerable portion of SFWST disposal research and significant advances have been made over the past years. The current international activities center on the following key research questions:

- **Engineered Barrier Integrity**: What is the long-term stability and retention capability of backfills and seals? 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? Is gas pressure increase and gas migration a concern for barrier integrity?
- **Near-Field Perturbation**: How important are thermal, mechanical, and other perturbations to a host rock (such as argillite/clay/shale, crystalline rock, and salt), and how effective is healing or sealing of the damage zone in the long term? How reliable are existing predictive models for the strongly coupled thermal-hydrological-mechanical and chemical behavior of clay and salt formations?
- **Flow and Radionuclide Transport**: What is the effect of high temperature on the diffusion and sorption characteristics of clays (i.e., considering the heat load from dual-purpose canisters)? What is the potential for enhanced transport with colloids? Can transport in diffusion dominated (i.e., clay, bentonite, salt) and advection dominated systems (i.e., fractured granite) be predicted with confidence?
- **Integrated System Behavior, Performance Assessment, and Site Characterization**: Can the early-time behavior of an entire repository system, including all engineered and natural barriers and their interaction, be measured and demonstrated? Can this integrated behavior be reliably predicted? Are the planned construction and emplacement methods feasible? Which characterization and monitoring methods are suitable for site selection and performance confirmation? How reliable are performance assessment models?

International collaboration has allowed engagement of U.S. researchers with the international waste management R&D community in terms of best practices, science advances, state of the art simulation tools, characterization and monitoring methods, performance assessment and confirmation approaches, lessons learned, etc. The joint R&D with international researchers, the worldwide sharing of knowledge and experience, and the access to relevant data/experiments from a variety of URLs and host rocks has helped SFWST researchers significantly improve their understanding of the current technical basis for disposal in a range of potential host rock environments. Comparison with experimental data has contributed to testing and validating predictive computational models for evaluation of disposal system performance in a variety of generic disposal system concepts. Comparison of model results with other international modeling groups, using their own simulation tools and conceptual understanding, have enhanced our confidence in the robustness of predictive models used for performance assessment. The possibility of linking model differences to choices in conceptual model setup provides guidance into “best” modeling choices and understanding the effect of model uncertainty. Access to international field testing also provides an opportunity to develop, test, and demonstrate new methods and workflows for site characterization and monitoring of deep geological disposal. International collaboration finally provides opportunities for training/educating junior staff well suited to move the U.S. disposal research program forward into the next decades. Promising avenues exist for further expansion of the international program.

This annual report describes the FY24 status of SFWST participation in international collaborative research activities on nuclear waste disposal in geologic formations. The focus of the report is on the description of opportunities that provide access to field data (and respective interpretation and modeling), and/or allow for participation in ongoing and planned field experiments. The report is an update to earlier annual reports summarizing SFWST’s international activities (Birkholzer, 2012; 2014; 2015; 2016; Birkholzer et al., 2017; 2018; 2019a; 2020; 2021; 2022; 2023).

2 STRATEGY FOR INTERNATIONAL COLLABORATION

Recognizing the benefits of international collaboration toward the common goal of safely and efficiently managing the back end of the nuclear fuel cycle, DOE's Office of Nuclear Energy (NE) and its Office of Spent Fuel and Waste Science and Technology (formerly Used Fuel Disposition, UFD) have developed a strategic plan to advance cooperation with international partners (UFD, 2012). The strategic plan lays out two interdependent areas of international collaboration (UFD, 2012). The first area is cooperation with the international nuclear community through participation in international organizations, working groups, committees, and expert panels. Such participation typically involves conference and workshop visits, information exchanges, reviews, and training and education. Examples include multinational activities, such as under the International Atomic Energy Agency (IAEA) (e.g., review activities, conference participation, and education), or the Nuclear Energy Agency (NEA, see Section 3.5) (e.g., participation in annual meetings, NEA's Clay, Salt and Crystalline Club, NEA's IDKM Group). DOE also actively supports several bilateral agreements for international information exchanges and other collaboration purposes. SFWST will continue participating in and/or supporting ongoing international collaborations in this first area, assess their benefits, and identify the need to expand and extend their scope. New activities and agreements may be developed with an eye toward the objectives and R&D needs of the United States (UFD, 2012).

The second area of international collaboration in the strategic plan involves active R&D participation of U.S. researchers within international projects or programs (UFD, 2012). Active collaboration means in this report that U.S. researchers work closely with international scientists on specific R&D projects relevant to both sides. Concerning the geologic disposal of radioactive waste, such active collaboration provides direct access to information, data, and expertise on various disposal options and geologic environments collected internationally over the past decades. Many international programs have been operating URLs in clay/shale, granite, and salt environments, in which relevant field experiments have been and are being conducted. Depending on the type of collaboration, U.S. researchers can participate in planning, performing, and interpreting experiments in these URLs, thereby getting early access to field studies without having *in-situ* underground research facilities in the U.S.

SFWST considers this second area, active international R&D, to be particularly beneficial to the program, helping to efficiently achieve the program's key disposal research goals, such as the short- and medium-term research objectives as described in Update of the Used Fuel Disposition Campaign Implementation Plan (FCRD-UFD-2014-000047, September 2014, Bragg-Sitton et al., 2014). For example, the Campaign Implementation Plan called for achieving a "comprehensive understanding of the current technical basis for the disposal of used nuclear fuel and high-level nuclear waste in a range of potential disposal environments to identify long-term R&D needs" and developing "advanced, predictive computational models, with experimental validation, for evaluation of disposal system performance in a variety of generic disposal system concepts and environments." It was decided in 2012 that the SFWST campaign priority should focus on advancing and utilizing such active international collaboration in disposal research. Coordinated by LBNL, a focused effort was made to collect information on international opportunities that complement ongoing disposal R&D within the SFWST, help identify those activities that provide the most significant potential for substantive technical advances, interact with international organizations and programs to help advance specific collaborations, and initiate specific R&D activities in cooperation with international partners.

Active collaboration can be achieved under different working models. One option is informal peer-to-peer interaction with international R&D organizations. Many U.S. scientists involved in SFWST research activities have close relationships with their international counterparts, resulting from workshops and symposia meetings or active R&D collaboration outside SFWST. Continued SFWST support for the participation of U.S. researchers in relevant international workshops, meetings, and conferences. and symposia help foster discussion and expand such relationships. Other working models for active international collaboration require that DOE becomes a formal member in multinational initiatives. Since the launch of the international disposal research collaboration program in 2012, DOE has joined six international cooperation initiatives as a formal partner: the Mont Terri Project (since 2012), the DECOVALEX initiative (since 2012), the CFM Project (2012 through 2015), the Full-scale High-Level Waste Engineered Barriers Experiment Dismantling Project, FEBEX-DP (2012 through 2015), the SKB (Swedish Nuclear Fuel and Waste Management) Task Forces (since 2014), and recently the HotBENT Project, a high-temperature EBS experiment at the Grimsel Test Site in Switzerland (since 2018). These provide access to field data from URLs and/or allow participation in ongoing and planned URL field experiments. Section 3 of this report gives a comprehensive overview of these initiatives and describes the various opportunities arising from DOE's membership. Outside of the above initiatives, SFWST scientists also collaborate with individual international disposal programs, which may or may not require formal bilateral agreements. Section 4 presents an overview of the international disposal programs that are open to bilateral collaboration with U.S. researchers. Both sections describe relevant collaboration opportunities that the SFWST campaign has already engaged with as well as others that are promising for potential engagement.

The benefit of international collaboration needs to be evaluated and periodically reevaluated in the context of the open R&D issues that can be addressed through collaborative scientific activities. Section 5 points out that a reassessment of SFWST's international research portfolio has been conducted routinely to respond to changing research priorities and boundary conditions and the development of new opportunities for collaboration. The section starts with the first planning exercise for the international portfolio conducted by SFWST in FY11 and FY12, which led to the initial selection of a set of R&D activities that align with current goals, priorities, and funded plans of SFWST and follows with a description of annual re-planning activities. A thorough "deep dive" reassessment was conducted in FY18 and FY19 as part of a broad SFWST campaign roadmap update, described in Sevougian et al. (2019). The purpose of this roadmap update was to summarize the progress of ongoing generic disposal R&D activities since 2012, to re-assess R&D priorities, and to identify new activities of high priority, such as R&D on disposal of dual-purpose canisters (DPCs) which now contain a significant fraction of the Nation's commercial spent fuel activity. In FY20, the DOE requested to develop a formal plan for activities in the disposal research in SFWST for the next 5-year period, which resulted in a strategic guidance document, updated regularly, that includes a 5-year direction for the international collaboration tasks (Sassani et al., 2020). Updates of this 5-year plan were developed in 2021 and 2023 (Sassani et al., 2021; 2023). In Section 5, results from these recent reassessments are briefly described and plans for better alignment of international modeling activities with new performance assessment modeling are discussed.

Section 6 summarizes key international collaboration research activities conducted by SFWST researchers in FY23. The descriptions of such research activities are kept very brief, as much more detailed information is provided in several referenced feeder reports. The section is structured by scientific challenge area (e.g., "Coupled Processes and Alterations in Bentonite-Based Engineered Barrier Systems, or "Coupled Processes in Salt"), whereas Sections 3 and 4 are structured by collaboration opportunity. Each research activity in Section 6 provides a pointer back to the specific international initiative or bilateral cooperation described in Section 3 and 4 that has provided the opportunity for collaboration.

3 MULTINATIONAL COOPERATIVE INITATIVES

This section gives a comprehensive overview of international cooperation initiatives that foster active research collaboration with other international disposal programs, provide access to field data (plus respective interpretation and modeling), and may allow participation in ongoing and planned field experiments in URLs. DOE is currently a formal partner in several of these initiatives, namely the Mont Terri Project (Section 3.1), the DECOVALEX initiative (Section 3.2), the HotBENT Project at the Grimsel test Site (Section 3.3), and the SKB Task Forces (Section 3.4). Table 3.1-1 lists the international waste disposal organizations participating in these initiatives, clearly demonstrating the high level of cooperation between nuclear nations. The section also describes selected initiatives that DOE is not currently participating in but might consider joining (e.g., Grimsel Test Site experiments other than HotBENT, SKB Prototype Repository retrieval).

Section 3.5 briefly touches on international collaboration initiatives organized by the NEA, where (except for the NEA Horonobe International Project, HIP) our engagement is less focused on active collaboration and more on exchanging information and shared approaches. Finally, Section 3.6 describes opportunities for cooperation with the upcoming EURAD-2 European Commission collaborative program, which will start a new round of repository R&D work in the Fall of 2024 through 2029.

Table 3.1-1. Participation of international programs in multinational initiatives related to URLs: Status FY24.

Nuclear Nation	Organizations	DECOVALEX 2023 and 2027	Mont Terri	HotBENT	SKB Task Forces
Belgium	SCK/CEN		x		
	FANC		x		
Canada	NWMO	x	x	x	x
	CNSC	x			
China	CAS	x			
Czech Republic	SURAO	x		x	x
France	ANDRA		x		
	IRSN		x		
	Total		x		
Finland	POSIVA				x
Germany	BASE	x	x		
	BGE	x	x	x	
	BGR	x	x	x	x
	GRS		x		
	BMWi/KIT				x
	Helmholtz Ass.	x	x		
	DynaFrax	x			
Japan	JAEA	x	x		x
	CRIEPI		x		x
	Obayashi		x	x	
	NUMO			x	
Netherlands	COVRA	x			
Rep. of Korea	KAERI	x			x
	KIGAM	x			
Spain	ENRESA	x	x	x	
	CIEMAT				
Sweden	SKB				x
	SSM	x			
Switzerland	NAGRA		x	x	x
	ENSI	x	x		
	ETH		x		
	swisstopo		x		
Taiwan	TaiPower	x			
United Kingdom	NWS	x	x	x	x
	Shell		x		

3.1 MONT TERRI PROJECT

3.1.1 INTRODUCTION TO THE MONT TERRI PROJECT

The Mont Terri Project is an international research project for the hydrogeological, geochemical, and geotechnical characterization of a clay/shale formation suitable for geologic disposal of radioactive waste (Zuidema, 2007; Bossart and Thury, 2007). The project was officially initiated in 1996 and has been conducted in a clay-rock underground rock laboratory, which lies north of St-Ursanne in northwestern Switzerland. The URL is ~300 m below the surface in argillaceous claystone (Opalinus Clay). The rock laboratory resides in and beside the security gallery (initially the reconnaissance gallery) of the Mont Terri motorway tunnel, which was opened to traffic at the end of 1998. The rock laboratory consists of the security gallery with small niches excavated in 1996, Gallery 98, with five lateral niches excavated in 1997-1998; a gallery for the EZ-A experiment, excavated in 2003; Gallery 04 with 4 lateral niches excavated in 2004, and Gallery 08 with side galleries for the Mine-by Test and Full-scale Emplacement Experiment excavated in 2008 (Figure 3.1-1). An additional tunnel excavation was conducted between 2018 and 2020, significantly expanding the URL and providing ample space for additional experiments. More information can be found at https://www.mont-terri.ch.

The Mont Terri Project operates as a collaborative program providing open access to an existing URL and the results of investigations. The research program consists of individual experiments divided into annual project phases. The Swiss Federal Office of Topography, swisstopo, helps conduct the operation and maintenance of the rock laboratory and provides operational management and experimental support. Organized as a consortium, the partner organizations (currently 23) fund the experiments and the related technical work. Partner organizations can select to conduct experiments, participate in experiments conducted by others, and have access to all project results from past and ongoing efforts, which are available in reports and a project-owned web-based database. Planning, steering, and financing is the responsibility of all partners participating in each experiment.

Over the years, the organizations involved in the Mont Terri Project have provided substantial financial investments. Additional support has been given by the European Community and by the Swiss Federal Office for Science and Education. The Mont Terri Project has been very successful, and a wide range of experimental studies on clay/shale behavior (including backfill/buffer behavior) have been conducted. In recognition of the Mont Terri Project's 20th anniversary in 2016, a Special Issue of the Swiss Journal of Geosciences provided a range of publications describing key experiments and achievements of the Mont Terri Project (Bossart et al., 2017).

In 2011, the DOE leadership recognized that membership in the Mont Terri Project could be highly beneficial to SFWST's R&D mission, and in early 2012, decided to formally apply for membership. DOE's partnership started officially with Phase 18 of the project, which ran from July 1, 2012, through June 30, 2013. Today, DOE is one of 22 partners (plus swisstopo as a managing organization) from nine countries of the Mont Terri Project, namely from Switzerland (ENSI, Nagra, ETH), Belgium (SCK/CEN, FANC), Canada (NWMO), France (Andra, IRSN, Total), Germany (BASE, BGE, BGR, GRS, Helmholtz Association), Japan (OBAYASHI, JAEA, CRIEPI), Spain (ENRESA), United Kingdom (Shell, NWS), and the U.S. (Chevron, DOE). Participation in the project provides unlimited access to operating URLs in a claystone environment, with several past and ongoing experiments that are highly relevant to SFWST's R&D objectives. The DOE's membership has given SFWST researchers access to relevant field data and projects resulting from all past Mont Terri phases. More importantly, SFWST researchers have been working collaboratively with international scientists on selected experimental studies, including the design, characterization, modeling, and interpretation aspects of field experiments. DOE also has an opportunity to propose and eventually conduct its experiments at the Mont Terri URL, which could be an option for project future phases.

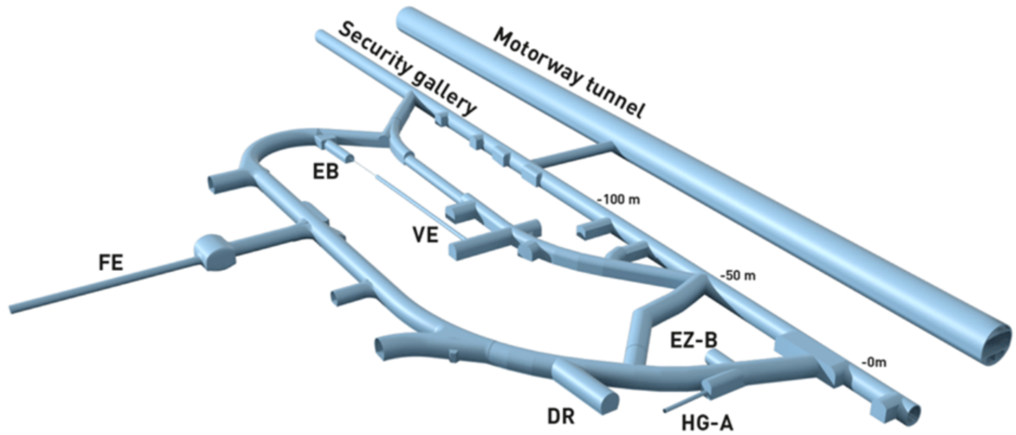


Figure 3.1-1. 3D schematic of the Mont Terri URL with side galleries and drifts. This schematic does not show the recently finalized expansion of the URL. Abbreviations point to some of the key experiments conducted at Mont Terri.

Figures 3.1-2 and 3.1-3 show an overview of key experiments conducted at the Mont Terri URL as described in the 2016 Special Issue of the Swiss Journal of Geosciences (see Bossart et al., 2017 and other publications in the Special Issue). The timeline in Figure 3.1-2 places these experiments in the context of relevance to different phases in the lifetime of a repository: (1) experiments related to initial conditions and repository construction, (2) experiments related to early-time perturbations, (3) experiments related to transient- to late-time post-closure phase of a repository. For comparison, the figure also shows two features that are important for the repository evolution: (1) the temperature variations in the buffer (red curve) indicating the thermal loading of the disposal system canister emplacement, and (2) the transient changes in buffer saturation (blue curve) indicating the slow process the bentonite buffer reaching fully saturated conditions. Figure 3.1-3 shows the same key experiments in a plan.

Many experiments shown in Figures 3.1-2 and 3.1-3 are long-running tests that have carried on into the current Phase 26 (July 2021 through June 2022) of the Mont Terri Project and that will continue into future project phases. While a few experiments at Mont Terri are relevant to other subsurface applications, such as geologic carbon sequestration, most activities are related to the geologic disposal of radioactive waste or have cross-cutting relevance, including waste disposal. Since 2012, DOE has engaged in several such experiments, such as the *in-situ* Heater Experiment in Micro-tunnel (HE-E) Heater Test, the Engineered Barrier (EB) Experiment, the Mine-by Test, the Gas Path through Host Rock and Seals Experiment (HG-A), and the DR-A Diffusion, Retention, and Perturbation Experiment. Currently, SFWST scientists are participating in, or utilizing data from, three major tests at Mont Terri: the FE Heater Test, the FS and FS-B Fault Slip Experiments, and the Cement-Clay Interaction (CI-D) Experiment. General information about the experiments in which DOE is currently involved is given in Sections 3.1.2 through 3.1.4, and summaries of SFWST research activities related to these experiments are provided in Section 6. Almost all these field experiments are further supported by laboratory and modeling tasks.

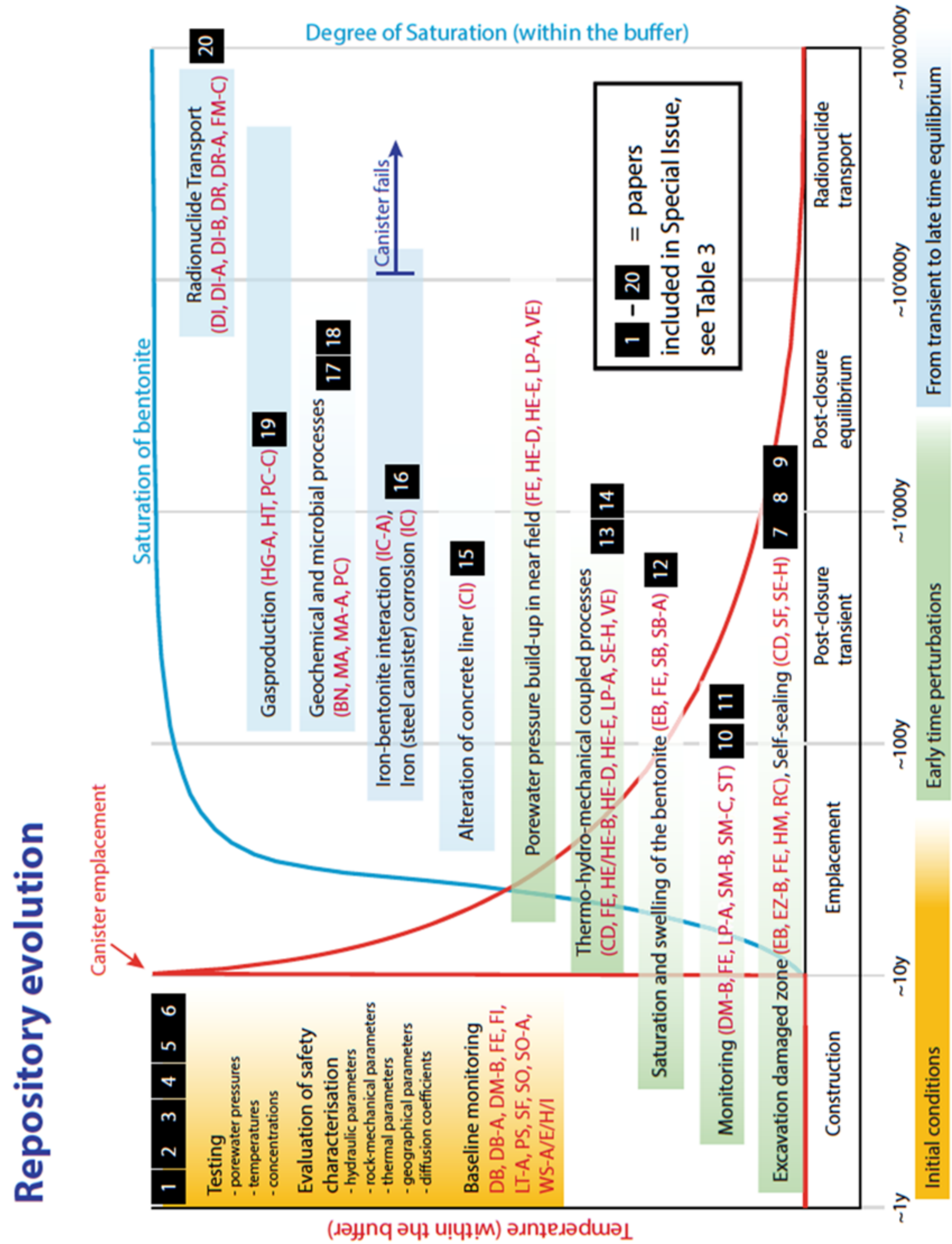
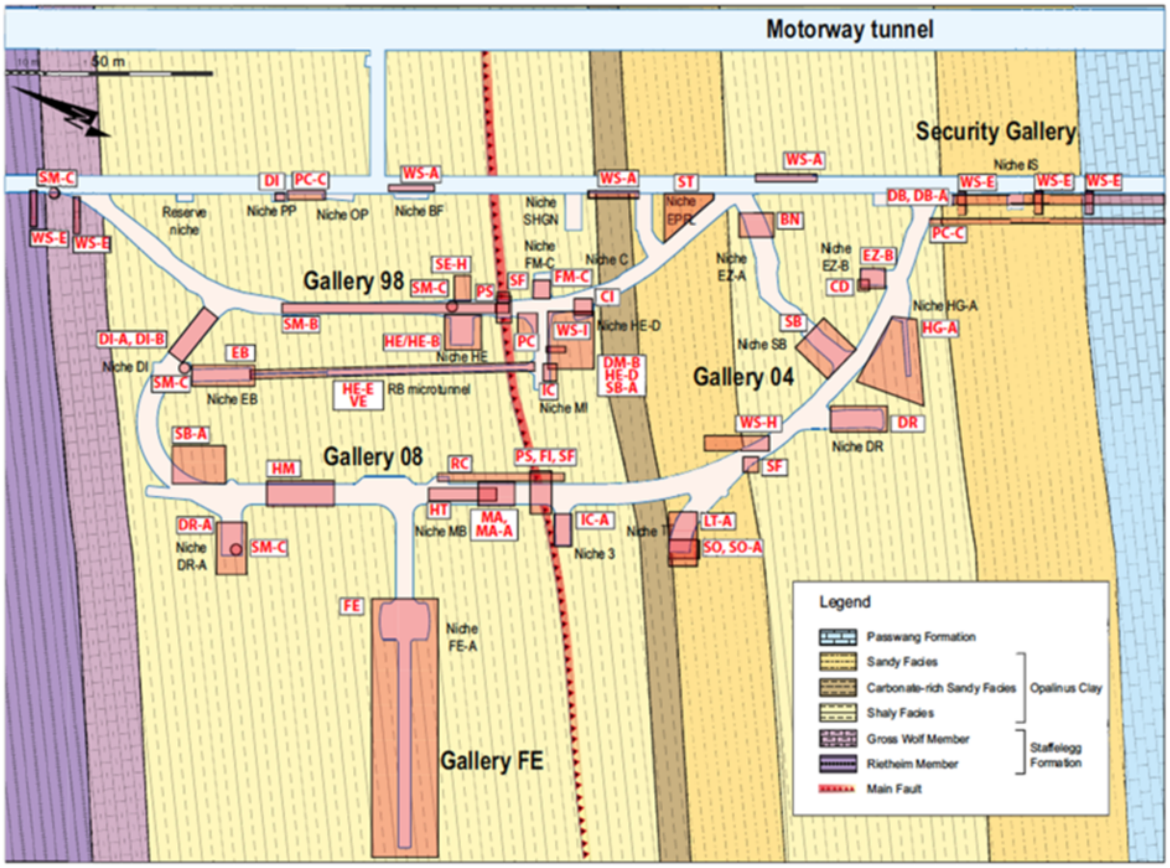


Figure 3.1-2. Major Mont Terri URL experiments as described in Bossart et al. (2017). Only a subset of the full Mont Terri experimental portfolio is shown here. Numbers 1-20 (in black) point to publications in the 2017 Special Issue of the Swiss Journal of Geosciences (Vol. 110, pp. 1-412).



BN	Bitumen-nitrate-clay interaction
CD	Cyclic deformations
CI	Cement-clay interaction
DB	Deep inclined borehole through the Opalinus Clay
DB-A	Porewater characterisation-Benchmarking
DI	Diffusion in rock
DI-A	Long-term diffusion
DI-B	Long-term diffusion
DM-B	Long-term deformation measurements
DR	Diffusion and retention experiment
DR-A	Diffusion, retention and perturbations
EB	Engineered barriers
EZ-B	Fracture generation
FE	Full scale emplacement demonstration
FI	Fluid-mineral interactions in Opalinus Clay during natural faulting and heating
FM-C	Flow mechanism (tracer)
HE/HE-B	Heater experiments I and II
HE-D	THM behaviour of host rock (heater test)
HE-E	In-situ heater test in VE microtunnel
HG-A	Gas path host rock & seals
HM	Experimental lab investig. on HM-coupled properties & behavior Opalinus Clay
HT	Hydrogen transfer
IC	Iron corrosion of Opalinus Clay
IC-A	Corrosion of iron in bentonite
LP-A	Long-term monitoring of parameters (porewater pressures)
LT-A	Clay properties, analyses of labtesting
MA	Microbial activity in Opalinus Clay
MA-A	Modular platform for microbial studies
PC	Porewater chemistry
PC-C	Gas porewater equilibrium
PS	Petrofabric and strain determination
RC	Rock mass characterisation
SB	Selfsealing barriers clay - sand mixtures
SB-A	Borehole sealing experiment
SE-H	Self-sealing with heat (Timodaz)
SF	Self-sealing of tectonic faults
SM-B	High resolution seismic monitoring
SM-C	Permanent nanoseismic monitoring
SO	Sedimentology of Opalinus Clay
SO-A	Palynology of the Opalinus Clay
ST	Seismic transmission measurements
VE	Ventilation test
WS-A/E/H/I	Porewater profiles, wet spots

Figure 3.1-3. Plan view of the Mont Terri URL with key experiments and a selected list of relevant experiments. Gallery FE indicates the area of the FE Heater test, which is currently the largest subsurface heater experiment worldwide (Bossart et al., 2017). This schematic does not show the recently finalized expansion of the URL.

The collaborative nature of the Mont Terri project allows for efficient initiation and planning of new experimental works. At each Technical Meeting held in January or February every year, partner organizations may give a brief presentation of any new proposed work to be conducted annually in the upcoming Mont Terri project phases. The proposing partners present the technical scope and merits of the proposed work, give a rough cost estimate, and then invite other partner organizations to consider joining the new task. In some cases, the proposing partners could provide a direct financial contribution to the experiment, and in other cases, they may invite partners to conduct monitoring or modeling analysis that complements their proposal. They will then write a short project description before the next Mont Terri Steering Committee Meeting (typically held a few months following the Technical Meeting), where ongoing and new experiments are selected. The experimental program for the next project phase is then finalized, including the consideration of the financial contributions of partners, at the second Steering Committee Meeting held just before the start of the new phase. Partners can be found if the proposed work aligns with the interests of other Mont Terri organizations. It is important to note that the existing infrastructure at Mont Terri makes developing and conducting experiments very easy, even if the proposing partner is far from the URL. swisstopo can handle many of the organizational details if needed, and a long list of experienced contractors is available to conduct the actual experimental work.

In the Spring of 2018, the Mont Terri Project started construction on a significant extension of the URL, which has now been finalized and provides an important additional working space for new large-scale experiments. As shown in Figure 3.1-4, an extension of the URL was achieved via a tunnel loop excavated in a southwestward direction. Before and during the excavation, the project leads held several planning exercises to brainstorm how the new experimental space should be used. About 45 proposals for new experiments were submitted, of which about 60% were related to nuclear waste. Some of these have been initiated or are in the final planning stages. These offer promising opportunities for DOE to engage (see some examples in Section 3.1.5).

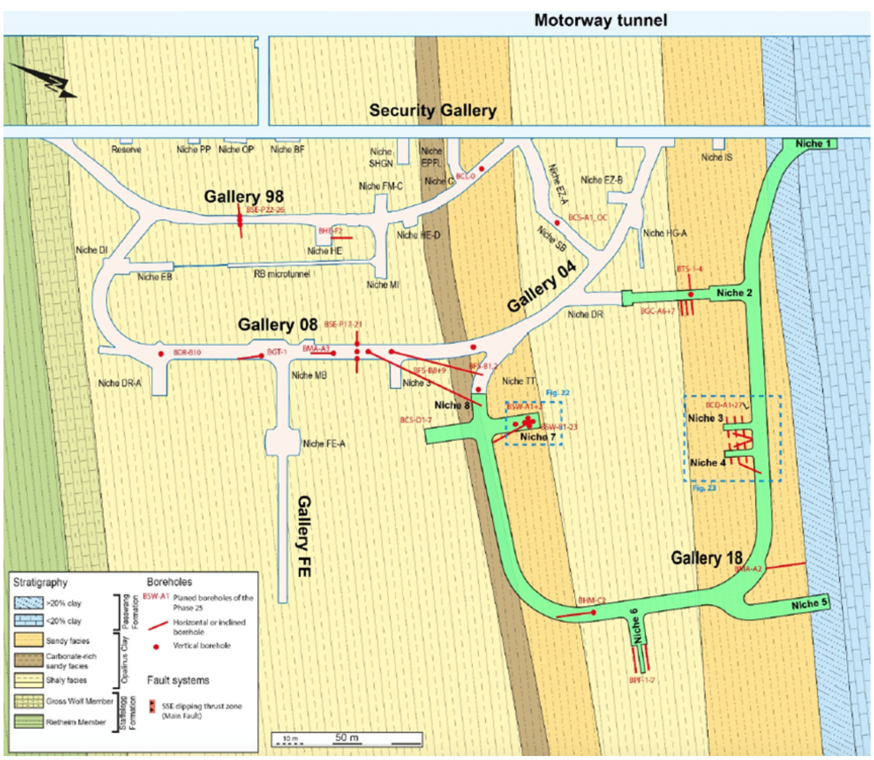


Figure 3.1-4. Plan view of the Mont Terri URL after extension of the URL in mostly southwestward direction. The green coloring shows the added tunnels and niches.

3.1.2 FE HEATER TEST

The Full-Scale Emplacement Experiment (FE Heater Test) is one of the largest and will likely be the longest-duration subsurface heater test ever conducted. This heater experiment has been designed by Nagra as a long-term test for the performance of geologic disposal in Opalinus Clay, with a focus on both EBS components and host-rock behavior. Mont Terri partners collaborating with Nagra in this experiment are Andra, BGR, GRS, NWMO, and DOE starting from July 2012. As shown in Figures 3.1-5 through 3.1-7, the FE Heater Test is conducted in a side niche and gallery at Mont Terri, excavated along the claystone bedding plane for this purpose, with 50 m length and about 2.8 m diameter. Heating from emplaced waste is simulated by three heat-producing canisters of 1,500 W maximum power. A sophisticated monitoring program was planned and implemented, including dense pre-instrumentation of the site for *in-situ* characterization, dense bentonite buffer, host rock instrumentation, and extensive geophysical monitoring. A THM modeling program is conducted parallel with the testing and monitoring activities.

After years of preparation and construction, including installation of the heaters, the bentonite buffer, and instrumentation, the heaters were ramped up to full power by March 1, 2015 (Figure 3.1-8). During the preparation phase, predictive THM models of the anticipated FE Heater Test behavior were developed by some project partners (among them SFWST scientists from LBNL), for the support of the design and instrumentation planning, as well as for the comparison of “blind predictions” with measured THM effects. A staged heating approach was employed in which the three heaters were turned on subsequently (Figure 3.1-9). This ensured that the models for predicting the maximum temperature in the buffer were validated against early temperature data from one heater before running all three heaters simultaneously.

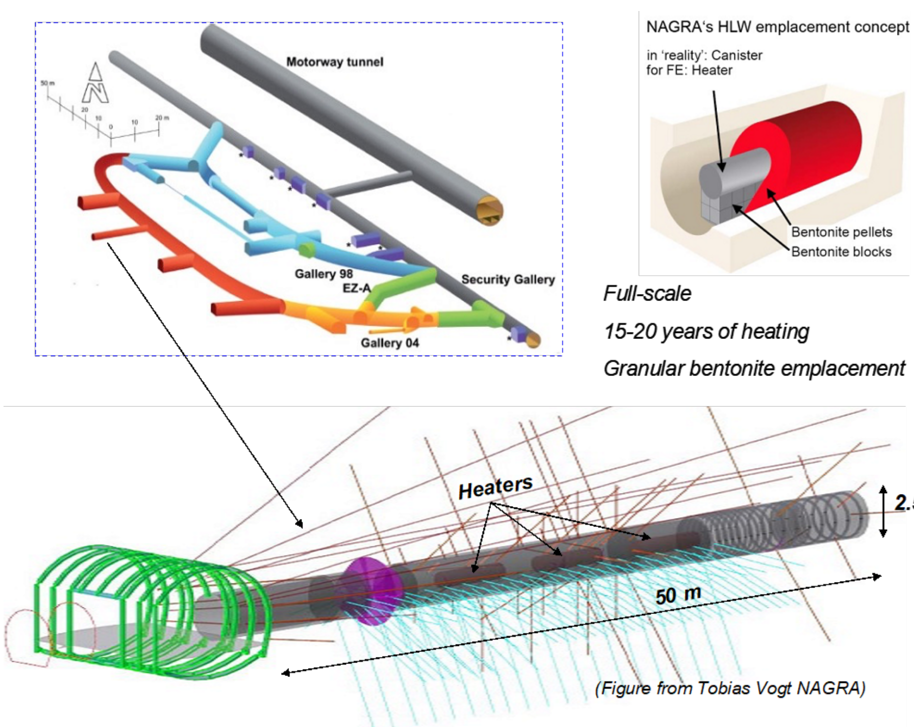


Figure 3.1-5. FE Heater Test at Mont Terri URL: experiment setup and borehole layout (Zheng et al., 2015).

To date, after almost nine years of heating, the experiment has provided valuable data for the validation of THM coupling effects regarding the processes in the host rock, while accounting for (and examining) the expected conditions in the emplacement tunnel (temperature, saturation, stress pressure, and swelling pressure). Due to the 1:1 scale of the experiment, it is possible to achieve realistic temperature, saturation, and stress gradients. The experiment also allows for the testing of backfilling technology with granular bentonite, as well as an application of lining technology with shotcrete, anchors, and steel ribs. It provides ample opportunity to examine the suitability of various monitoring methods. Processes examined in the test cover many aspects of the repository evolution, such as the Excavation Damage Zone, or Excavation Disturbed Zone (EDZ) creation and desaturation during tunnel excavation and operation (including ventilation for about one year), reconsolidation of the EDZ, re-saturation, thermal stresses, and thermal pore-pressure increase after backfilling and heating (heating and monitoring period > 10 years).

SFWST researchers and their international partners have been working on the interpretative modeling of the first several years of monitoring data from the FE Heater test. Data from the FS Heater Test have recently been utilized in a THM modeling task in the DECOVALEX-2023 initiative, with multiple international modeling teams participating, including LBNL and SNL. See Section 3.2.3.3 in this report for a brief description of the DECOVALEX-2023 modeling task and Section 6.3.2 for a summary of the findings of the comparative modeling study. For more detailed information on LBNL's and SNL's modeling work, see Section 4 of Rutqvist et al. (2024a) and Section 2 of Hadgu et al. (2024).

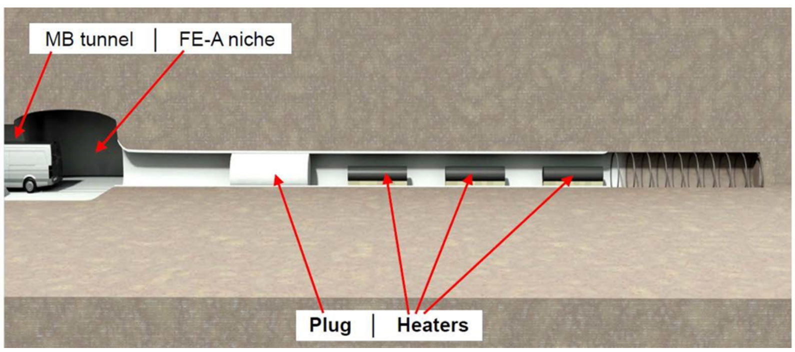


Figure 3.1-6. FE Heater Test: Side view of the experiment setup and the heater layout (Garitte, 2010).

Figure 3.1-7. View from the FE gallery into the heater tunnel during the final installation (Bossart, 2014).

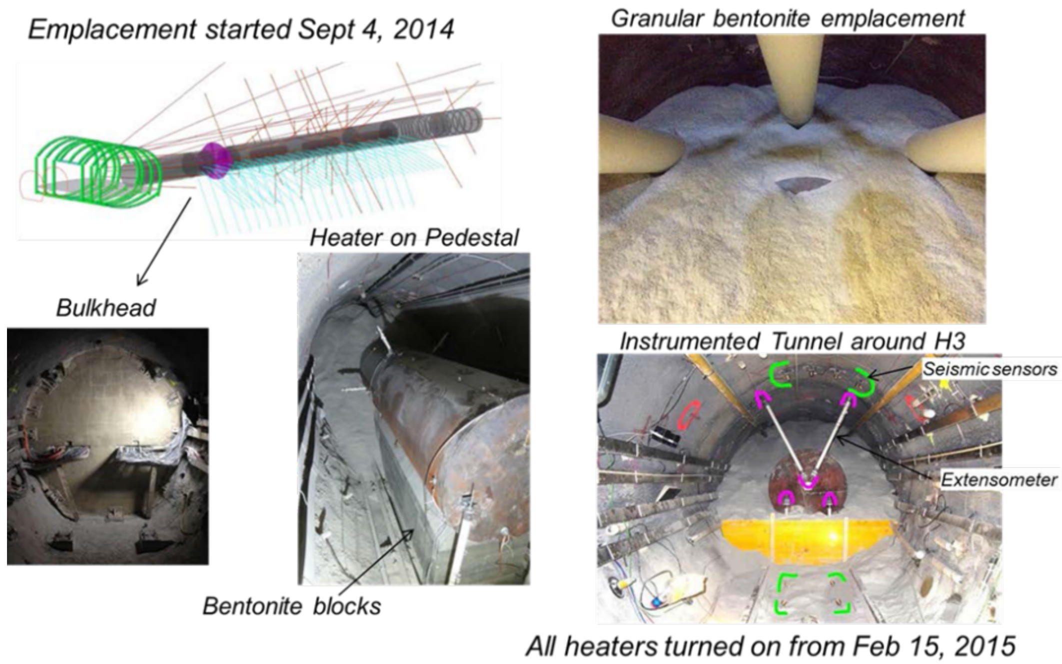


Figure 3.1-8. Images from the construction and installation of heaters, bentonite backfill and plugs (Zheng et al., 2016).

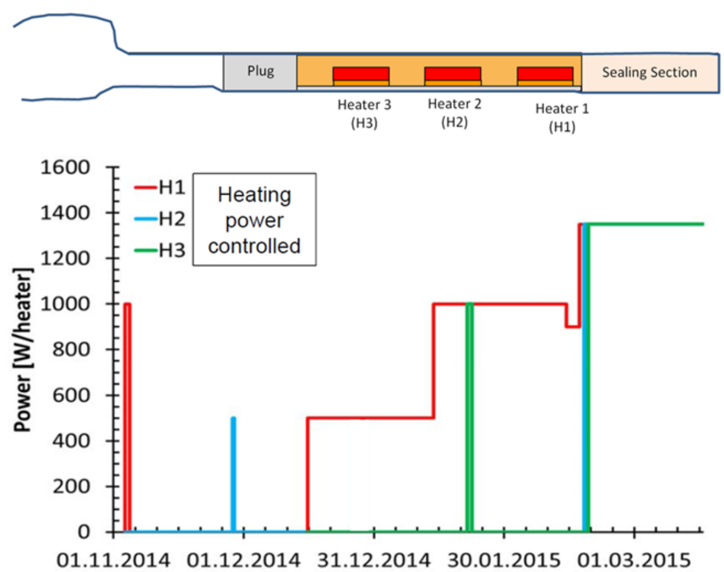


Figure 3.1-9. Heat power applied to Heaters H1, H2, and H3 during the start-up of heating at the Mont Terri FE experiment.

3.1.3 FS, FS-B, FS-C AND FS-F FAULT ACTIVATION EXPERIMENTS

As shown in Figures 3.1-10 and 3.1-11, the Mont Terri URL is transected by an intermediate-scale fault, which provides intriguing opportunities for *in-situ* testing of fault activation and fault slip caused by pressure and stress changes. In geologic repositories for nuclear waste, such changes could be triggered, for example, by thermal stresses or gas pressure increases. The LBNL team led the Mont Terri first fault activation experiment in 2015, referred to as the Fault Slip (FS) Test, which was aimed at understanding (1) the conditions for slip activation and stability of clay faults and (2) the evolution of the coupling between fault slip, pore pressure and fluids migration. Results obtained by the experiment are crucial for defining mechanisms of natural and induced earthquakes, their precursors, and risk assessment, as well as for a better understanding of the possibility of the loss of integrity of natural low permeability barriers. Recent studies suggest that the slow slip of faults may be a dominant deformation mechanism of shale during hydraulic stimulation or other extensive subsurface injection activities (Zoback et al., 2012). The same mechanism may be necessary in case of stress perturbation, which may reactivate a pre-existing fault and eventually enhance rock permeability, for example, due to drilling a network of underground galleries for radioactive waste emplacement. A similar concern may be the fault slip caused by the increase of pore pressure due to heating from the high-level waste or gas generation due to steel corrosion. Hence, the possibility of increasing permeability caused by fault slip and generation of potential pathways in the host rock or in an upper sealing formation could cause a significant risk to the long-term safety of a repository.

The key idea of the 2015 FS experiment at Mont Terri was to conduct controlled fault-slip experiments via localized pressurization in a packed-off section of a borehole drilled through the Mont Terri main fault zone (Figures 3.1-10 and 3.1-11). Water was injected between inflatable packers at increasing flow rates to progressively decrease the effective stress until fault destabilization occurs while monitoring injection flow rate, pore pressure, fault slip, and normal displacement evolution from the stable to the unstable fault states. Monitoring was performed with a new device called the Step-Rate Injection Method for Fracture *In-situ* Properties (SIMFIP) probe (Guglielmi et al., 2013a,b), which is capable of measuring slip velocities and slip deformation at unprecedented spatial resolution. The probe allows for simultaneous high-frequency monitoring of full 3D-deformations of the borehole wall, fluid pressure, and injection flow rate within a 1.5 m long injection chamber set between two inflatable packers. The accuracy of measurements is very high, with a measurement resolution of 10^{-6} for deformations, 10^{-3} Pa for pressure, and 0.1 L/min for flow rate. Two experimental test sequences were conducted using the SIMFIP probe in the main fault zone in May and October 2015. Both test sequences involved injection into different test intervals in two separate boreholes (Figure 3.1-12). The experiments demonstrated that fault activation and slip resulted in drastic (yet short-term) permeability increases in the initially very low-permeability fault. Results from the 2015 test were utilized as a modeling task in a previous phase of the DECOVALEX initiative, referred to as DECOVALEX-2019.

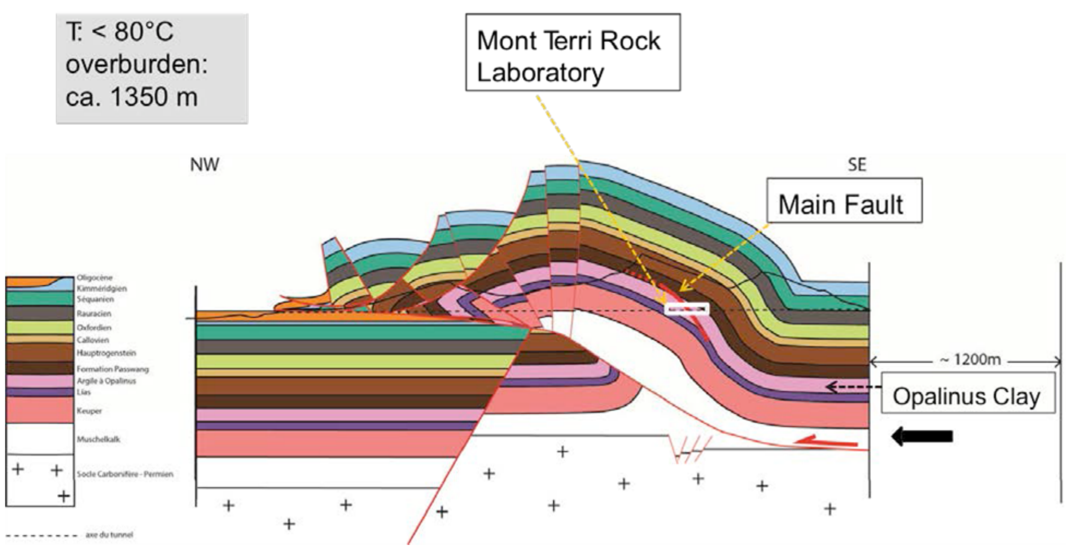


Figure 3.1-10. Geologic setting showing Mont Terri URL and location of the main fault (Guglielmi et al., 2015).

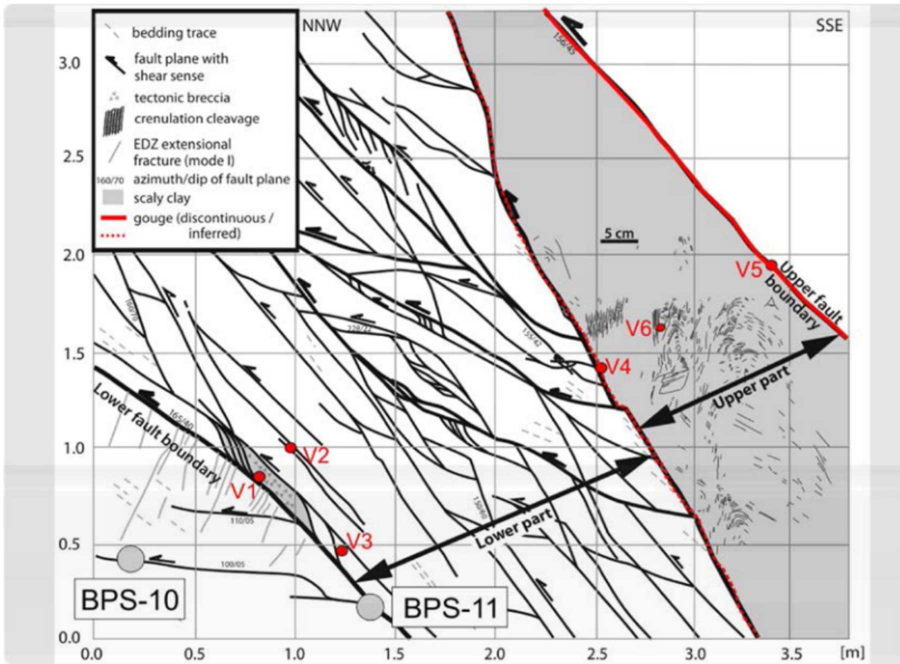


Figure 3.1-11. Detailed fault geometry at Mont Terri (Guglielmi et al., 2015).

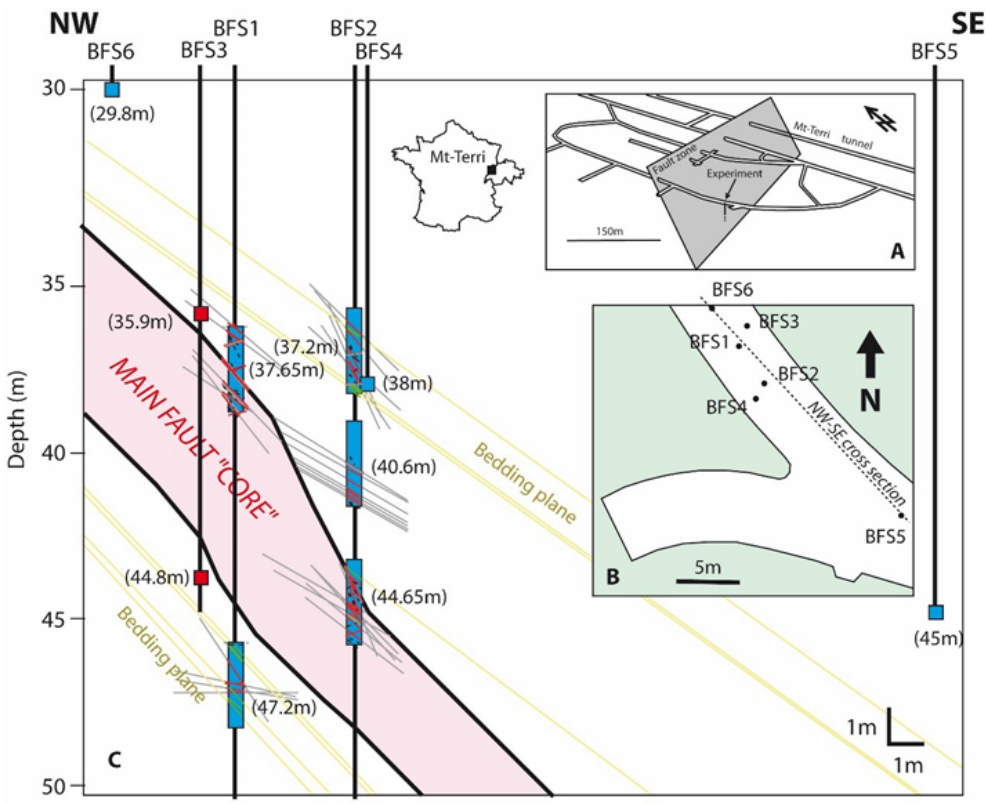


Figure 3.1-12. Test intervals across the Mont Terri Main Fault (red squares are seismic sensors, blue squares are piezometers, blue rectangles are injection and monitoring intervals); (a) experiment location in Mont Terri URL; (b) map of the borehole geometry in the FS experiment zone; and (c) cross-section showing the different testing intervals.

Several Mont Terri partner organizations, including DOE, partnered in 2018 to plan and develop a larger-scale fault testbed of 70 m by 70 m by 70 m for follow-on experiments, referred to as FS-B (Imaging the Long-Term Loss of Faulted Host Rock Integrity) and most recently FS-C (Understanding Fault Slip and Subsequent Sealing Processes in OPA). FS-B and FS-C feature a similar controlled-injection fault reactivation program as the previous FS test but activate a much larger fault patch and use an upgraded version of the SIMFIP tool. The FS-B/FS-C testbed is located near the location of the previous FS experiment, at the intersection between Gallery 4 and the new tunnel of the rock lab extension (Figure 3.1-15). The objective of FS-B/FS-C is to understand longer-term impacts and processes during and after the fault activation; therefore, several activation and monitoring periods have been planned and executed over a multi-year period. FS-B/FS-C also involves active seismic imaging of fluid flow and stress variations using a cross-well design that straddles the activated fault. In 2019 and 2020, the partners concluded all preparatory activities for FS-B, including the drilling of several boreholes into and along the fault and the installation of the monitoring equipment. A first fault reactivation test was conducted in November 2020, followed by repeat experiments in 2021, 2022, and 2023. Figure 3.1-13 shows the overall testbed geometry, and Figure 3.1-14 shows the setup of tilted boreholes that straddle the fault and allow for cross-well seismic imaging with a semi-continuous monitoring approach referred to as Continuous Active Seismic Source Monitoring (CASSM), in combination with fiber optics cables for distributed acoustic and strain sensing (DAS and DSS).

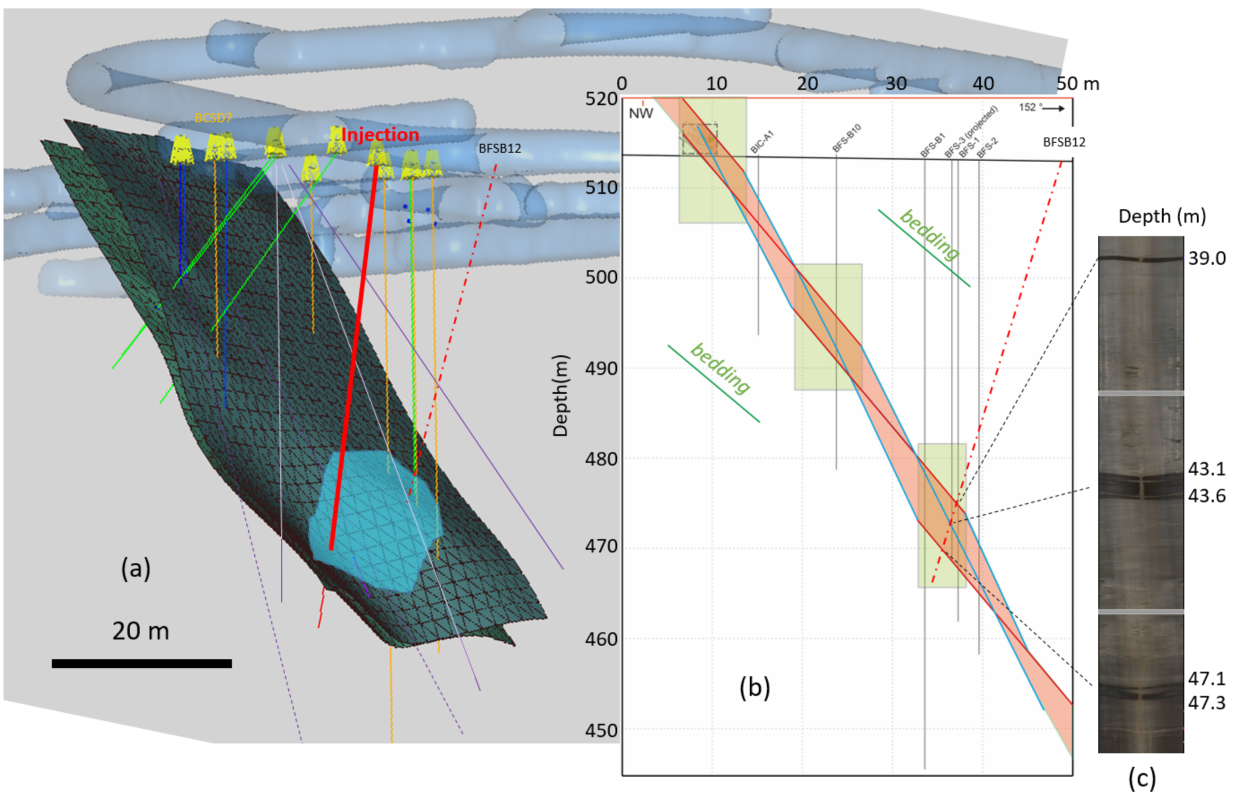


Figure 3.1-13. 3D setup of the FS-B/FS-C experiment. (a) Main fault top and bottom surfaces. (b) Geological cross-section showing the schematic internal structure of Asperities. (c) Post 2021 injection experiment coring through the Main Fault showing three wet zones corresponding to preferential flow paths created during the experiment.

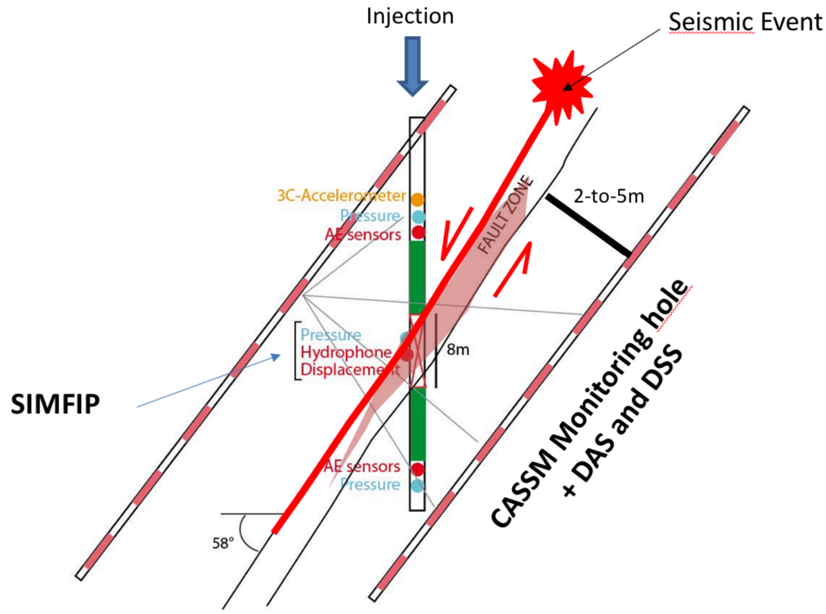


Figure 3.1-14. Vertical cross-section showing a schematic of tilted boreholes for cross-well geophysical monitoring of the dynamic fault behavior upon activation.

As mentioned above, mentioned above, the first fault stimulation experiment in the larger testbed took place on November 21, 2020. Six consecutive injections were successfully conducted in a borehole at 40.4 m depth below the Mont Terri galleries through a 1 m long interval set across the top of the Main Fault zone. The fault hydraulically opened when injection pressure was between 5 and 6 MPa. At some point during the injection cycles, when the cumulated injected volume reached 178 liters, a hydraulic connection was established between the injection and a monitoring borehole in Gallery 2008, located 15–18 m away along the fault strike. No clear hydraulic connection was observed in other boreholes intersecting the fault, indicating an apparent heterogeneity in the fault leakage behavior. Results of the time-lapse seismic imaging of CASSM conducted during the first FS-B injection demonstrated that changes in p-wave velocities across the fault are measurable and that such changes are correlated to changes in effective stress and deformations induced during and after the injection. The seismic imaging also suggests the leakage volume is local within the fault zone. Instantaneous changes in the seismic signals relate to fracture opening, while delayed changes might highlight some irreversible shear damage following activation. The repeat experiments conducted in 2021 and 2023 confirmed many of the observations from the 2020 test, such as the same fault opening pressure and a similar leakage path within the fault. The FS-B/FS-C testing and advanced HM modeling of experimental observations have resulted in a much-improved understanding of fault reactivation and permeability enhancement in low-permeability shales (e.g., Cappa et al., 2022).

In addition to monitoring the short-term active injection as described above, the FS-B /FS-C testbeds allowed for measuring the long-term hydromechanical behavior of the fault after activation, particularly the sealing of the fault and the evolution of fault permeability. This was done by conducting a series of small-volume pulse-test injections over time and using the observed pressure increase to back-calculate the changes in fault transmissivity. These pulse tests were repeated roughly every month over one year. The analysis of pressure pulse tests showed a fast drop in transmissivity from 3.2×10^{-7} m^2/s during the high-pressure activation phase to 1.8×10^{-9} m^2/s five days after activation, followed by a slow decrease of ~1.6×10^{-9} m^2/s per year during the following eight months (Figure 3.1-15). 200 days after activation, the fault transmissivity remained about two orders higher than the initial fault transmissivity before activation. To interpret these observations, LBNL scientists then tested different fault transmissivity versus time relationships. They used the best-fit models to predict how long it would take to complete sealing of the activated fault. While uncertainties are acknowledged, their predictions indicate that complete sealing may take at least 50 years, even under the most favorable conditions. These are significant findings for the performance assessment of a clay repository.

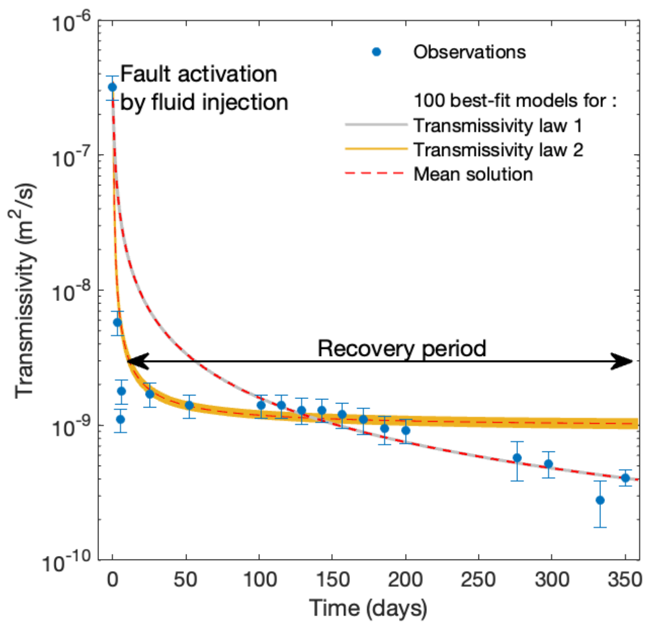


Figure 3.1-15. Evolution of predicted fault transmissivity over time compared to experimental data estimated from the series of pulse tests. Experimental results are shown as blue dots with error bars taken at ±20% to account for possible uncertainty of measurements. Two fault transmissivity laws are deployed, shown in gray and orange. Source: Rutqvist et al. (2024a, Section 8.2.3.2).

SFWST scientists have been key participants in the FS, FS-B, and FS-C activities, contributing to the tests' design, monitoring, analysis, and modeling. A summary of FY24 research activities is given in Section 6.7 of this report. More details can be found in Rutqvist et al. (2024a). FY24 research activities include improved interpretation and physics-based modeling of fault injection and long-term sealing behavior (Section 8 in Rutqvist et al., 2024a), complemented by novel machine learning approaches to predict the HM response of an argillite fault (Section 6 in Rutqvist et al., 2024a).

In FY24, LBNL researchers and international partners also started planning a new phase of fault slip studies using the Mont Terri testbed to study whether the heat emanating from decaying waste might create high thermal stresses to reactivate the fault. The new FS-F Fault Heating experiment will create a controlled thermal stimulation of the fault by deploying 3 m long heaters in boreholes drilled a few meters from the fault zone at about 40 m depth below the Mont Terri galleries. The temperature will be raised in steps up to about 110°C, a reasonable limit for all monitoring instruments and a high limit for temperature increase in the natural barrier of a waste repository. A feasibility heat test will be conducted in the existing FS-B/FS-C instrumented volume to benefit from the already installed multi-modal monitoring network that includes DTS, DSS, DAS, RFS-DSS optical fibers, local fault pore pressure and 3D displacement monitoring, active seismic imaging and passive seismic monitoring (Figure 3.1-16). The feasibility test is scheduled for late 2024. Results from this feasibility test will guide the design and execution of a dedicated THM fault activation test to be conducted in FY25.

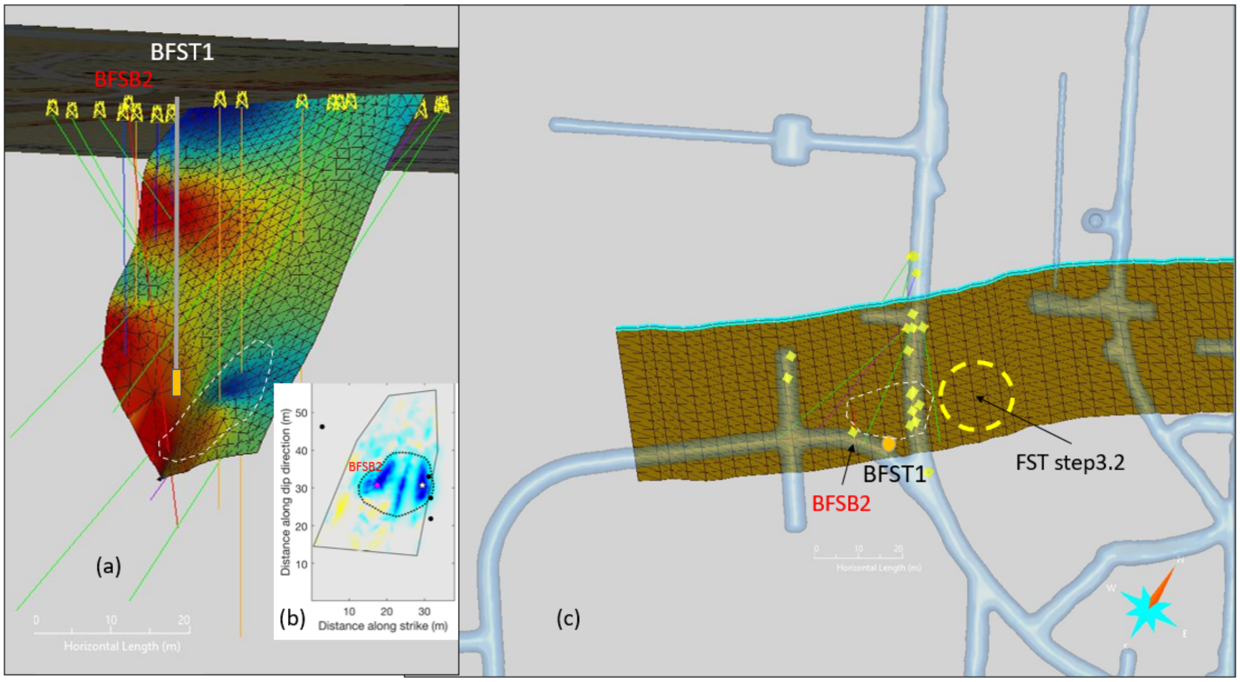


Figure 3.1-16. Location of the FS-F experiment in the FS-B/FS-C testbed. (a) Feasibility test by heating a 3 m long section at the bottom of borehole BFST1 that would be drilled outside the fault in the hanging wall. (b) Leakage pathway imaged in FS-B experiments. BFST1 would heat the fault between the BFSB2 injection hole and the monitoring hole shown as the white star on the right of the p-waves image. (c) A larger map of the Main Fault shows where a larger-scale Fault Heating experiment could be deployed. Source: Rutqvist et al. (2024a, Section 8.6).

3.1.4 CI-D EXPERIMENT

The Cement Clay Interaction (CI-D) Experiment at Mont Terri is linked to the long-term cement-interaction (CI) Experiment conducted in Gallery 98 since about 2007. As shown in Figure 3.1-17, CI was set up with two vertical boreholes with multiple segments with bentonite and concrete/cement materials interacting with the argillite host rock. Since then, several sampling campaigns have been conducted in 2009, 2012, 2015, and 2017, where slanted boreholes were carefully drilled into the vertical boreholes to retrieve core materials with interfaces between bentonite, concrete/cement, and clay rock. These past campaigns aimed to characterize these interfacial regions about time-dependent mineralogical, chemical, or textural changes.

The idea of CI-D was to go beyond the characterization of interfaces with various imaging approaches to directly measure *in-situ* the transport properties and processes across the interfaces. In May 2019, a water cocktail with radionuclide tracers was released in a slanted pilot borehole drilled into the vertical borehole in a Portland cement/concrete section. The tracer cocktail has since been allowed to migrate outwards mainly by diffusion across the interface and into the argillite host rock. Overcoring the affected rock volume with cement-claystone interfaces was conducted from October to December 2023. The cement-claystone interfaces retrieved from these cores have interacted for over 16 years. Analysis of the samples is expected to be complete in late 2024. Results from CI-D will provide valuable answers to questions about the impact of an aged concrete/claystone interface on the diffusive transport of water and solutes, i.e., whether a “skin” may form which may impede radionuclide transport (a beneficial effect) or cause delays in bentonite saturation (an unwanted effect).

In 2019, the CI-D project initiated a joint modeling effort in which SFWST scientists from LBNL joined in FY21. Starting with 1D radial and 2D axisymmetric hydro-chemical simulations, the LBNL modeling team has now developed and applied a full 3D dual continuum model in CrunchClay in which electrostatic effects in the electric double layer are explicitly resolved. See Section 6.2.4 of this report for a summary, and for more detailed information, see Section 9 of Rutqvist et al. (2024a). A direct comparison of the simulated interfacial reactions with the results of the overcoring of the cement-claystone interfaces is planned for FY25.

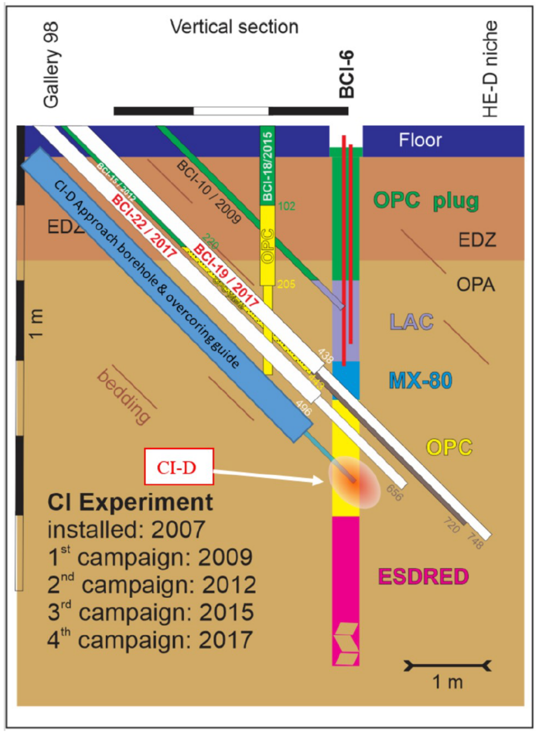


Figure 3.1-17. Schematic of CI-D experiment (Maeder and Martin, 2022). The CI-D overcoring borehole is approaching the zone of long-term interaction between OPC and the OPA. Note that the bedding within the OPA is parallel to the overcoring borehole and at an angle of about 45° from the contact with the cement plug. First, information from the overcoring is expected to be available in 2024.

3.1.5 OTHER SELECTED EXPERIMENTS AT MONT TERRI

3.1.5.1 SW-A SANDWICH EXPERIMENT

The SW-A Sandwich Experiment, conducted in a new niche in the extended rock lab (Gallery 18), is one of a few currently planned new experiments that address questions about suitable sealing approaches for a geologic repository, in this case, the sealing of vertical shafts in an argillite host rock. The Sandwich seal consists of highly conductive equipotential layers placed in alternation with sealing layers to obtain a more homogeneous re-saturation of the seal. The system was successfully tested at the small and medium lab scale, demonstrating that the alternating layers of sealing segments and equipotential segments adsorb potential seal bypass and fingering, as well as high hydraulic loads. SW-A involves a large-scale field experiment to test the sandwich seal system in a natural rock environment (Figure 3.1-18). Two experimental shafts of 1.2 m diameter have been excavated. The first (primary) shaft has been entirely backfilled as planned (i.e., equipped with the designed alternating sandwich seals), and extensive instrumentation of the shafts and surrounding rock was installed. The seals in the first shaft were hydrated since May 2021 via slanted boreholes from the shaft bottom. After some initial problems with leakage along some cables, the pressurization progressed as planned, as the seal evolution and rock response were monitored in terms of saturation, pore pressure, stress, and deformation. Shaft 1 has been operating at constant injection pressure since early 2022. The second (backup) shaft installation started in September 2022, considering the experience from the primary shaft. Shaft 2 has been operating since early 2023.

The lead organization for the SW-A experiment, the German GRS, brought the data from the experiment into the new Sandwich task of the current DECOVALEX-2027 phase that was just initiated in the Spring of 2024 (see Section 3.2.3.4). The topic of developing and testing suitable sealing elements for tunnels, shafts, and boreholes in different host rocks is essential to the SFWST campaign.

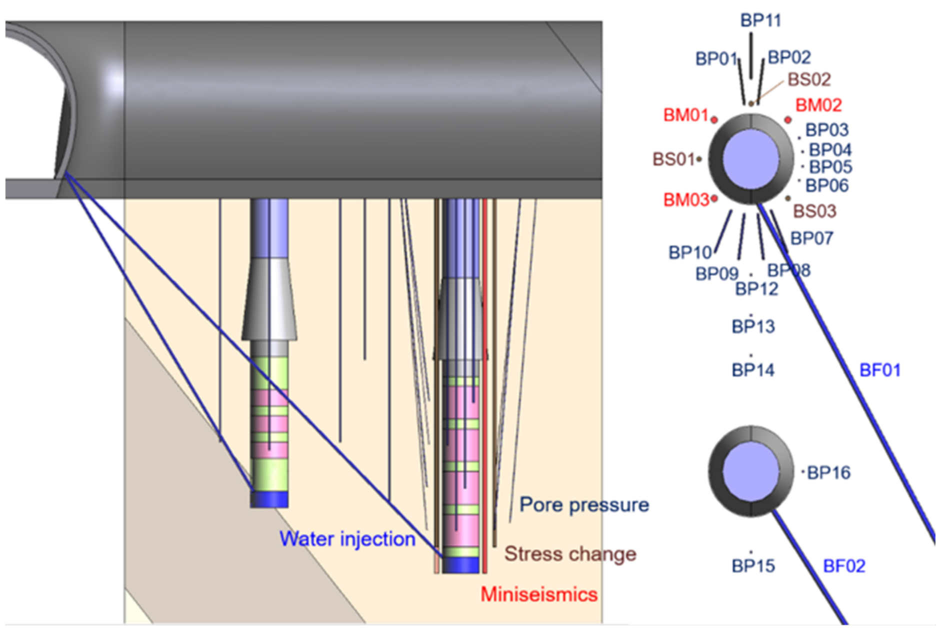


Figure 3.1-18. Design of SW-A experiment with two vertical shafts and planned monitoring approach (Hesser and Wiezcorek, 2020).

3.1.5.2 GT EXPERIMENT

The GT Experiment aims to evaluate gas transport models and the behavior of clay rocks under gas pressure. Conventional theory suggests that as the gas pressure increases up to the capillary entry pressure, the gas phase starts to displace water from the pore system. Upon further gas pressure increase, the system will be successively drained as the gas phase displaces the wetting phase from smaller pores. When finally, a continuous non-wetting phase has developed (gas breakthrough) through the pore network, viscous gas flow is initiated. However, in initially saturated clay-rocks with extremely narrow interparticle spaces, the capillary threshold pressure required to initiate gas flow can be too large for the gas to penetrate and desaturate the clay (Horseman et al., 1999). In a clay-rich host formation, there is significant uncertainty as to whether gas can escape through the host rock without the pressure rising to a level where fractures occur and create preferential pathways, potentially leading to groundwater transport.

The GT Experiment focuses on the characterization of the physical phenomena describing the gas transport and its mechanical interaction with the surrounding barriers. The goal is to further understand the creation of micro- and macro-fractures and whether they could be a concern for the long-term safety of a repository. The experiment is conducted in a stepwise approach, starting with laboratory experiments using samples of Opalinus Clay (OPA) from Mont Terri to the field-scale rock laboratory experiment that was designed based on the laboratory experiment results. In 2019, samples of OPA taken from Mont Terri were tested in a triaxial permeameter cell and analyzed with the help of micro-imaging techniques. Strain data obtained during these experiments (see example in Figure 3.1-19) support process understanding, helping to differentiate between visco-capillary and dilatant gas flow mechanisms. Laboratory tests were performed parallel and perpendicular to bedding to evaluate anisotropy in the material response. Meanwhile, the installation of the field experiment is progressing: all monitoring wells and the central injection well have been drilled (Figure 3.1-20). After an initial hydraulic testing campaign, the experiment is now underway and will last for about two years. Gas injection below the fracking pressure follows a step-rate hydraulic testing sequence. Injection is conducted into several packed-off intervals and the response of the formation is monitored in a series of parallel observation boreholes arranged in a radial array. It is planned to model the experiment with numerical codes considering both visco-capillary and dilatant processes to elicit which behavior predominates. The GT Experiment has been included as a modeling subtask in the new HyMAR task of the current DECOVALEX-2027 phase (see Section 3.2.3.2).

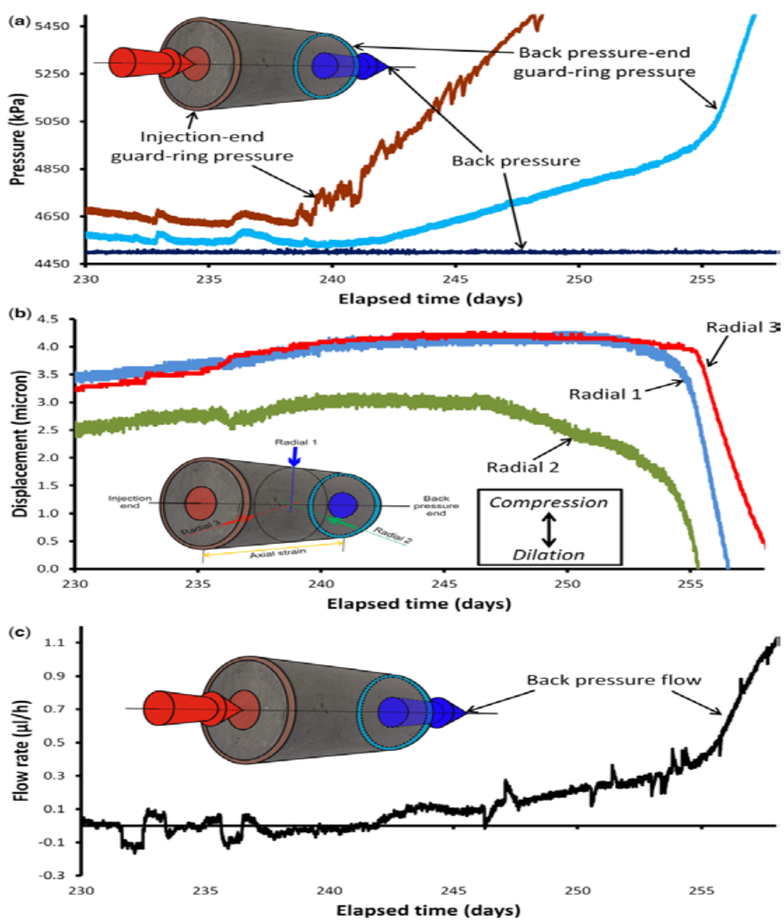


Figure 3.1-19. Data from a triaxial test report by Cuss et al. (2014) showing the response of a claystone sample at the onset of gas flow: (a) pressure response; (b) radial deformation; (c) outflow from the sample.

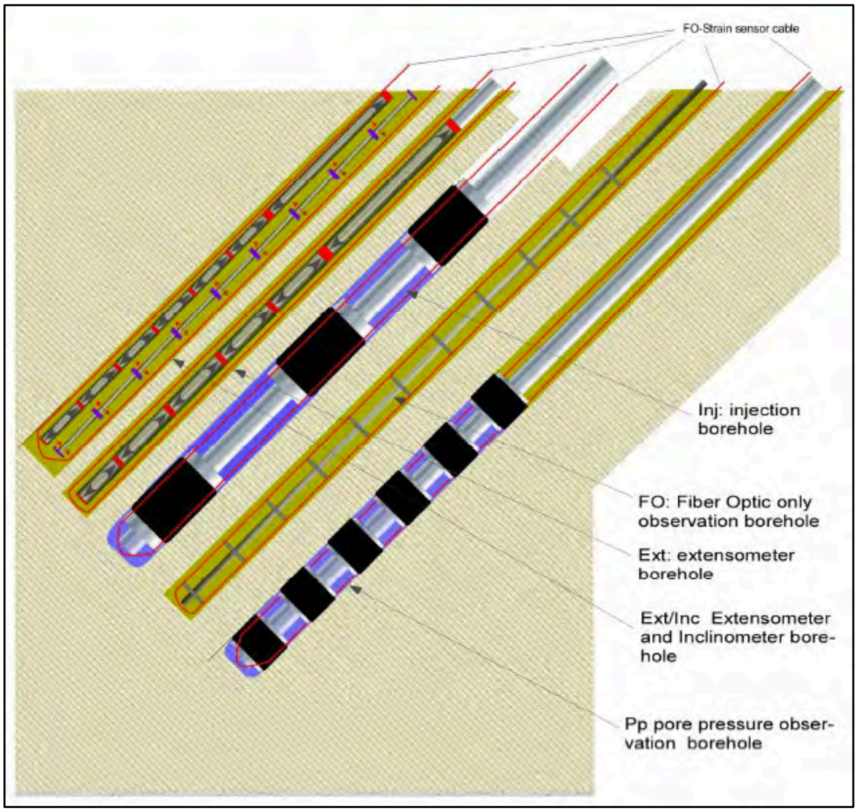


Figure 3.1-20. Schematic showing the field test design with central gas injection borehole surrounded by monitoring boreholes.

3.1.5.3 MA-A EXPERIMENT

Microbial processes can significantly impact the long-term performance of a disposal site. In the near-field and regarding engineered barrier behavior, microbial activity (MA) can enhance the corrosion of containment systems like the waste packages; MA may also alter the migration properties of radionuclides in the near-field rocks. MA may have beneficial effects at later stages because microbes can consume the hydrogen gas generated from the long-term corrosion of canisters. The MA-A experiment at Mont Terri aims to answer questions related to the characterization of microbial communities in the pore water of the Opalinus Clay. The experiment is set up to allow surface access to collect samples and decoupling the downhole from the surface equipment. The technical design is as follows: Borehole BMA-A1 serves to obtain characteristics of unaltered Opalinus Clay porewater, including microbiota developed in the borehole since drilling. (Drilling was conducted using disinfected drills). Because only water lines are designed for an outflow of accumulated water, no disturbance of the developed microbiota is expected. When necessary, an inert argon gas phase was introduced using sterile filtered argon gas. Nearby, in the alcove next to the Mont Terri gallery, a laboratory space was designed with a glovebox to provide controlled anoxic conditions (Figure 3.1-21). Ease of accessibility enables the utilization of Opalinus Clay porewater for microbial analysis and scientific experiments. Because the design was focused on ensuring anoxic conditions (with oxygen sensors installed between the packer and the gallery ceiling, shielding of water lines, and the anoxic glovebox), experiments can be conducted under the realistic reducing environment of Opalinus Clay rock. SFWST researchers have considered participation in the analysis of MA-A data, but it has not been decided yet.

Figure 3.1-21. Borehole BMA-A1 (top) and glovebox in side alcove (bottom) of MA-A experiment.

3.1.5.4 DR-C EXPERIMENT

The DR-C Experiment is one of several experiments enabled by the recent rock lab extension. Installed in 2021 in the new Gallery 18, DR-C has the following objectives: (1) understand the *in-situ* diffusion behavior in Opalinus Clay in the presence of a thermal gradient, and (2) assess the *in-situ* effect of temperature and temperature gradients on the diffusion of selected radionuclides. Such assessment is essential for any radionuclide release scenario early enough to have radionuclide transport coincide with a thermal gradient, such as in certain early canister failure scenarios. The experimental setup includes a central injection borehole drilled vertically below a Mont Terri gallery, surrounded by a few monitoring boreholes nearby. Two separate experimental setups have been installed in the sandy facies of the Mont Terri rock lab, one heated setup with a temperature up to 80°C and one at ambient temperature as a reference test for comparison (Figure 3.1-22). A suite of laboratory diffusion experiments accompanies the field experiments. The lead organization for the DR-C experiment, the Belgium regulator FANC, has expressed interest in participation from additional partners, such as DOE. Still, no decision has been made in this regard by the SFWST campaign. Figure 3.1-23 shows the results of the first scoping simulations indicating the critical effect of bedding-plane-related anisotropy on tracer diffusion in the Opalinus Clay.

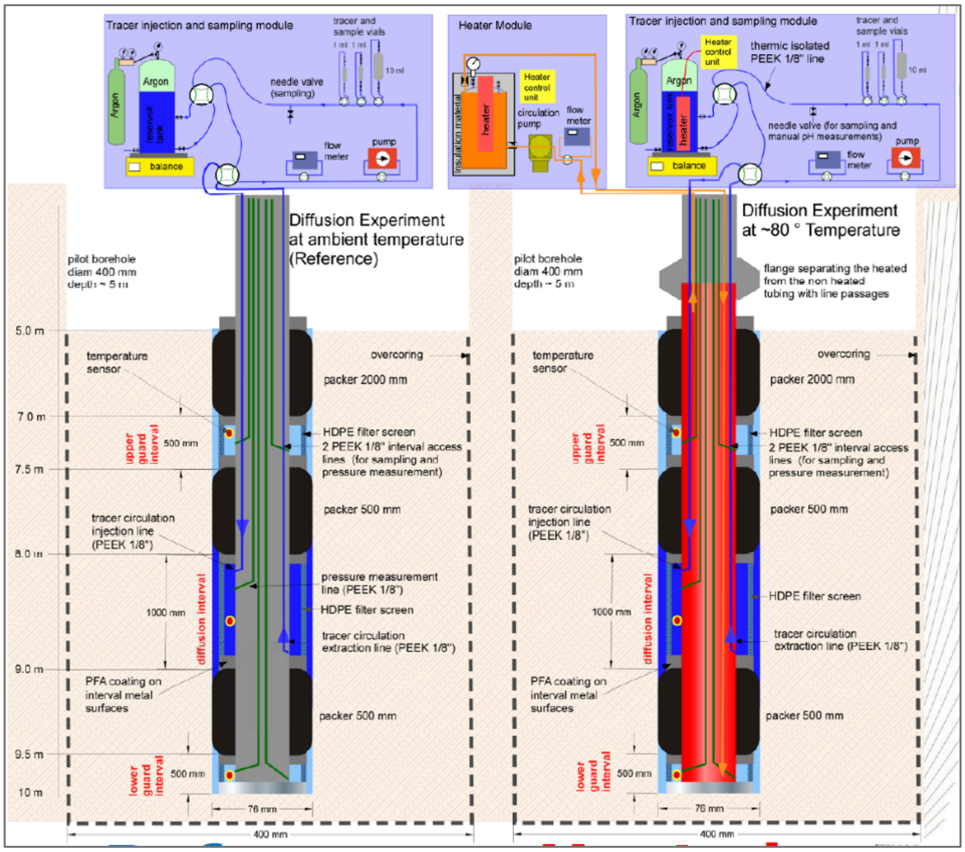


Figure 3.1-22. Schematic showing DR-C design with heated (right) and unheated(left) setups (Bernier and De Canniere, 2020).

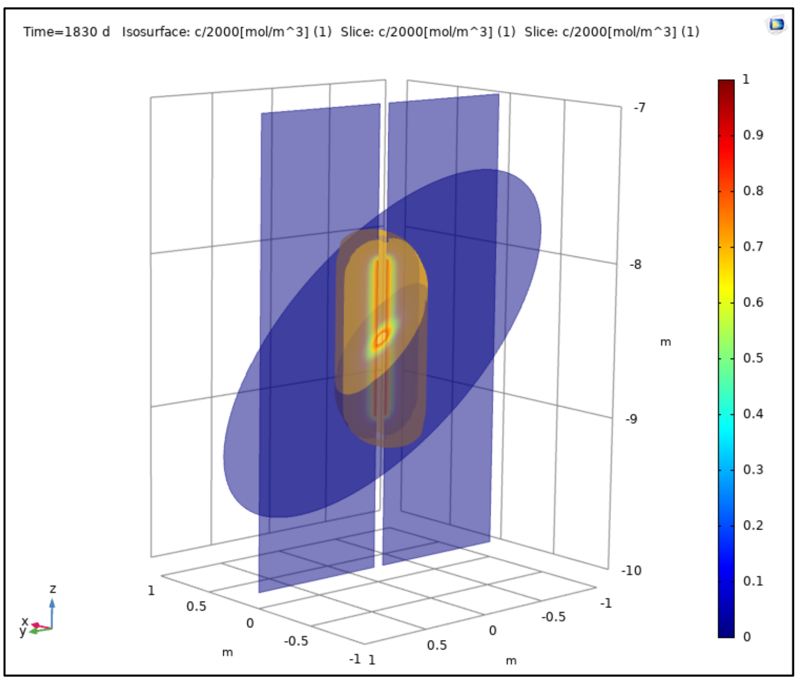


Figure 3.1-23. Scoping simulations of tracer diffusion in heated Opalinus Clay as per DR-C design (Bernier and De Canniere, 2020).

3.1.6 MONT TERRI SUMMARY

Benefits of Participation:

- Access to experimental data from the URL in clay/shale host rock, with many past, ongoing, and future experiments addressing various FEPs,
- Opportunity to participate directly in international research groups that conduct, analyze, and model experiments), and
- Opportunity to plan and conduct own research experiments

Status of Participation:

Effective July 1, 2012, DOE formally joined the Mont Terri Project as a partner organization. A substantial part of DOE's partnership fee was provided as an in-kind contribution by DOE researchers, i.e., by having SFWST researchers conduct work related to ongoing Mont Terri experiments. Specifically, the in-kind contribution of DOE included the participation of LBNL researchers in the design and prediction/interpretative modeling of the FE Heater Test, which is now a long-term ongoing research activity. In addition to the FE Heater Test, SFWST researchers have in prior years, participated in several other tests, such as the Mine-by Test, the HE-E Heater Test, the HG-A Experiment, and the DR-A Diffusion Experiment, and, as part of DECOVALEX-2019, have engaged in the collaborative modeling of the Engineered Barrier (EB) Experiment and the FS Fault Slip Test. In addition to the FE Heater Test, SFWST scientists are currently participating in, or utilizing data from, the FS-B/FS-C Fault Slip Experiment and the CI-D Cement-Clay Interaction Experiment. Under the umbrella of a new DECOVALEX-2027 initiative, SFWST modeling teams will work on data from the Sandwich and GT experiments. Overall, the participation of SFWST researchers in the Mont Terri Project has been highly beneficial.

Outlook:

SFWST researchers will stay involved in relevant experiments in the long-term FE Heater Test and keep abreast of new opportunities in the URL as they evolve. Eventually, DOE/SFWST may propose its experiments to be conducted at the site. The extension of the Mont Terri URL, finalized in 2020, provides significantly more space for new experiments, which ensures the long-term future of the collaborative Mont Terri Project. SFWST researchers should evaluate whether some of the many other relevant experiments conducted at Mont Terri (currently more than 50 ongoing experiments) offer important new scientific direction and are worth pursuing as new collaboration opportunities. Some selected opportunities are described above, such as the FS-F Experiment, MA-A Experiment and the DR-C experiment.

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3.2 DECOVALEX INITIATIVE

3.2.1 INTRODUCTION TO THE DECOVALEX INITIATIVE

The DECOVALEX Initiative is a multinational research collaboration for advancing the understanding and mathematical modeling of coupled THM and thermo-hydro-chemical (THC) processes in geologic and engineered systems associated with the geologic disposal of radioactive waste. DECOVALEX is an acronym for "Development of Coupled Models and their Validation against Experiments." Since 1992, the project has made substantial progress and played a key role in developing and validating advanced numerical models and in-depth knowledge of the complex THM and THC behavior of different host rock formations and buffer/backfill materials. The knowledge accumulated from this project, in the form of many research reports and international peer-reviewed journal and conference papers in the open literature, has been applied effectively in implementing and reviewing national radioactive waste management programs in the participating countries. The project has been conducted by research teams from many radioactive - management organizations and regulatory authorities from Canada, China, Finland, France, Japan, Germany, Spain, Sweden, the UK, the Republic of Korea, the Czech Republic, and the USA. A comprehensive overview of the project is provided on the DECOVALEX initiative website (www.decovalex.org).

The DECOVALEX initiative has generally been conducted in separate four-year project phases. Eight project phases were successfully concluded between 1992 and 2023, results of which have been published in a series of Special Issues in the International Journal of Rock Mechanics and Mining Sciences (Vol. 32(5) in 1995, Vol. 38(1) in 2001, and Vol. 42(5-6) in 2005), in the Journal of Environmental Geology (Vol. 57(6) in 2009), in the Journal of Rock Mechanics and Geotechnical Engineering (Vol. 5(1-2) in 2013), in the Journal of Environmental Earth Sciences (Vol. 77 in 2018), and in the International Journal of Rock Mechanics and Mining Sciences (Virtual Issue, DECOVALEX-2019, https://www.sciencedirect.com/journal/international-journal-of-rock-mechanics-and-mining-sciences/special-issue/10RM99KRN7V). The publications included in these Special Issues provide an in-depth overview of the collaborative research efforts conducted in the DECOVALEX initiative and how these have advanced the state of the art of understanding and modeling coupled THMC processes over a more than 25-year period. Summaries of the history and achievements of DECOVALEX are given in Tsang et al. (2009), Birkholzer et al. (2019b), and Birkholzer and Bond (2022).

Each DECOVALEX phase features a small number (typically three to seven) of modeling tasks important to radioactive waste disposal. Modeling tasks can be either Test Cases (TC) or Benchmark Tests (BMT). TCs are laboratory and field experiments conducted by one of the project partners and are then collectively studied and modeled by DECOVALEX participants. BMTs involve less complex modeling problems, often targeted at comparing specific solution methods or developing new constitutive relationships. Numerical modeling of TCs and BMTs, followed by comparative assessment of model results between international modeling teams, can assist both in interpreting the test results and testing the models used.

While code verification and benchmarking efforts have been undertaken elsewhere to test simulation codes, the model comparison conducted within the DECOVALEX framework is different because (a) the modeling tasks are often actual laboratory and field experiments, and (b) DECOVALEX engages model comparison in a comprehensive sense, including the modelers' choice of interpretation of experimental data, boundary conditions, rock and fluid properties, etc., in addition to their choice of simulators. Over the years, DECOVALEX has conducted collaborative modeling for tens of complex experiments, including several large-scale, multiyear field experiments (e.g., the Kamaishi THM Experiment in Japan, the FEBEX heater test at Grimsel Test Site in Switzerland, the Yucca Mountain Drift-Scale Heater Test, or the FE Heater Test at the Mont Terri URL). Thus, the project provides access to valuable technical data and expertise obtained by

DECOVALEX partner organizations; this is particularly useful in disposal programs that are starting their research on certain disposal or repository environments and have no URLs. DECOVALEX has a modeling focus but with a tight connection to experiments. Birkholzer et al. (2024) make a convincing case that the DECOVALEX initiative on modeling of coupled subsurface processes builds confidence in radioactive waste disposal. Table 3.2-1, extracted from this paper, describes the characteristics that according to the authors contribute to such confidence building.

Table 3.2-1. DECOVALEX characteristics contributing to confidence building in radioactive waste disposal (from Birkholzer et al., 2024).

Broad and comprehensive model comparison	Evaluation of alternative models used by multiple teams, comparison between models and with experimental data, discussion of model agreement and discrepancies, improvement of models, estimation of uncertainties.
Progressive Complexity of Tasks	Well-designed modeling tasks starting with simple benchmark tests before migrating to tasks of increasing complexity (e.g., complex experimental data sets, calibration, blind prediction).
Evaluating Scale Dependence	Focus on knowledge transfer between relevant scales: the micro-scale to study fundamental processes of importance, the meso-scale to examine process understanding in small field settings, the demonstration scale to confirm behavior of an entire emplacement unit, and finally the whole repository scale to assess long-term safety.
Close Integration of Experiments and Models	Modelers benefit from first-hand knowledge of experimental conditions and uncertainties. Experimentalists learn from comparative model evaluations and receive insights about the need for new or improved experiments. Both modelers and experimentalists benefit from enhanced conceptual understanding.
From Physics-Based Models to Reduced-Complexity Approaches	While the main focus is on physics-based modeling of coupled processes, DECOVALEX also evaluates the use of simplified models of reduced complexity that because of their fast simulation time are more amenable to probabilistic performance evaluations.
Knowledge Transfer Between Tasks	Tasks represent a broad portfolio of scientific challenges, designs, host rocks, and processes. Scientific lessons are transferred across tasks. New concepts and methods are developed through cross-fertilization.
Open Collaborative Environment Conducive to Knowledge Sharing	DECOVALEX emphasizes knowledge sharing through various means, including workshops, collaboration, publications, training, data and model sharing. Mentoring of PhD students and early-career researchers.

To participate in a project phase of the DECOVALEX initiative, interested parties—such as waste management organizations, regulatory authorities or research institutions—need to formally join the project and pay an annual fee for administrative and technical matters. In addition to this fee, participating (funding) organizations provide funding to their research teams to work on some or all the problems defined in the project phase. Representatives from the funding organizations form a Steering Committee that collectively directs all project activities.

DOE had been a DECOVALEX funding organization for several past project phases. In 2007, DOE decided to drop out due to the increasing focus on the license application for Yucca Mountain. When the radioactive waste disposal program shifted to other disposal options and geologic environments, a renewed DOE engagement with DECOVALEX was suggested in 2011 (Birkholzer, 2011) as a logical step for advancing collaborative research with international scientists. In 2011, DOE evaluated the benefits of joining the upcoming DECOVALEX phase from 2012 through 2015, referred to as DECOVALEX-2015. SFWST leadership realized that a renewed DECOVALEX participation would provide SFWST researchers access to relevant field data from international programs. They would allow them to work collaboratively with international scientists on analyzing and modeling these data. A decision was made in early 2012 that DOE would formally join the DECOVALEX initiative as a funding organization. SFWST researchers were involved in two of the three main modeling tasks in the DECOVALEX-2015 phase.

DOE has since remained an official and active funding organization in the DECOVALEX initiative. In 2016, Jens Birkholzer from LBNL became Chair of the DECOVALEX initiative. At the same time, DECOVALEX moved into the next project phase with seven modeling tasks for the years 2016 through 2019, referred to as DECOVALEX-2019 (Bond and Birkholzer, 2020; Birkholzer and Bond, 2022). DOE researchers participated in several of these DECOVALEX-2019 tasks, many of which involved data from URL experiments.

The most recently completed DECOVALEX phase (DECOVALEX-2023) started in April 2020 and ended in December 2023, again with DOE participation in multiple tasks and DOE leadership of two tasks. Brief descriptions of the seven tasks are given in Section 3.2.2. The currently active DECOVALEX phase, or DECOVALEX-2027, started in the Spring of 2024 and will run through the end of 2027. Information on the eight tasks for this new phase is provided in Section 3.2.3. SFWST scientists are heavily involved in DECOVALEX-2027, leading two tasks and participating in seven tasks.

3.2.2 DECOVALEX-2023

DECOVALEX-2023 is the most recent completed phase of the DECOVALEX initiative; this phase started in early 2020 and ended in late 2023. To identify suitable tasks for DECOVALEX-2023, the project organized several planning sessions during workshops in 2018 and 2019. At the end of this process, prospective funding organizations decided on seven relevant and interesting tasks to be included in DECOVALEX-2023. A total of 17 funding organizations participated in DECOVALEX-2023, including DOE. Jens Birkholzer from LBNL continued to serve as the Chair of the DECOVALEX initiative. A list of the DECOVALEX-2023 funding organizations is given in Table 3.2-2 below. The seven modeling tasks are briefly summarized in Table 3.2-3; more information is given in Sections 3.2.2.1 through 3.2.2.7. SFWST scientists served as task leads for two tasks, namely Task E and Task F, and they were involved in all but one of the seven tasks (with the participation of LBNL, SNL, and LANL scientists).

Table 3.2-2. Funding organizations involved in DECOVALEX-2023.

ANDRA	French National Radioactive Waste Management Agency	France
BASE	Federal Office for the Safety of Nuclear Waste Management	Germany
BGE	Federal Company for Radioactive Waste Disposal	Germany
BGR	Federal Inst. for Geosciences & Natural Resources	Germany
CAS	Chinese Academy of Sciences	China
CNSC	Canadian Nuclear Safety Commission	Canada
COVRA	Central Organisation for Radioactive Waste	Netherlands
DOE	Department of Energy	United States
ENRESA	Radioactivity and Radioactive Waste Management	Spain
ENSI	Swiss Federal Nuclear Safety Inspectorate	Switzerland
JAEA	Japan Atomic Energy Agency	Japan
KAERI	Korean Atomic Energy Research Institute:	Korea
NWMO	Nuclear Waste Management Organization	Canada
NWS	Nuclear Waste Services*	Great Britain
SSM	Swedish Radiation Safety Authority	Sweden
SURAO	Radioactive Waste Repository Authority	Czech Republic
TaiPower	Taiwan Power Company	Taiwan

* NWS was previously named Radioactive Waste Management (RWM)

Upon completion of DECOVALEX-2023, the initiative collaborated with ANDRA and LBNL to showcase its results in a large international symposium, the DECOVALEX Symposium on Coupled Processes in Radioactive Waste Disposal and Subsurface Engineering Applications. The symposium, held in Troyes, France on November 14-16, 2023, attracted about 200 participants who presented more than 100 oral and poster presentations, three keynotes, and a panel on the value of international collaboration. The scientific discussions, held both formally during the sessions and informally during breaks, advanced the state of the art in geologic disposal research about computational methods, lab experiments, and *in-situ* tests. Andra offered two technical site visits to the Meuse/Haute-Marne URL in Bure and the CSA/CIRES Waste Facilities on the last symposium day.

DECOVALEX-2023 is also the subject of a dedicated Virtual Special Issue in the Journal of Geomechanics for Energy and the Environment, guest-edited by Jens Birkholzer, DECOVALEX Chair, and Alex Bond, DECOVALEX Technical Coordinator. So far, the Special Issue has received more than 40 manuscripts that are currently in various publication or review stages.

Table 3.2-3. Modeling tasks for DECOVALEX-2023 (Bond and Birkholzer, 2019).

Task ID	Short Name	Title	Organization	Processes	Primary Material Type
A	HGFrac	Heat and Gas Fracturing	Andra	THM + gas	Argillite
B	MAGIC	Modeling Advection of Gas in Clays	BGS	HM + gas	Engineered Clay
C	-	THM Modeling of the FE Experiment	ENSI/Quintessa	THM	Argillite
D	-	Full-scale Engineered Barrier System Experiment at Horonobe URL	JAEA	THM(C)	Sedimentary
E	BATS	Brine Availability Test in Salt	DOE (SNL)	THMC	Evaporitic Salt
F	-	Performance Assessment (PA)	DOE (SNL)	PA – THMC	Crystalline and salt
G	SAFENET	Safety Implications of Fluid Flow, Shear, Thermal and Reaction Processes within Crystalline Rock Fracture Networks	UFZ, UoE, DynaFrax	THMC	Crystalline focus plus greywacke

3.2.2.1 HEAT AND GAS FRACTURING (HGFRAC) – TASK A

The overall objective of this DECOVALEX-2023 Task A was to improve the ability of models to predict the processes and mechanisms of fracture initiation and growth in claystone due to a rapid increase of heat or gas overpressure. Based on heat and gas fracturing tests conducted at the Bure URL in France, HGFrac enhanced the understanding of fundamental processes and improved capabilities for numerical modeling of these processes. Several tests had been designed and conducted by Andra to reach the rupture of claystone under either a rapid heat load or substantial gas pressure increase. The task was divided into two main sub-tasks that were undertaken in parallel, one on heat-driven and one on gas-pressure-driven fracturing. Both steps had a similar structure: (1) definition of conceptual models and initial benchmark exercises involving laboratory experiments, (2) blind prediction and numerical reproduction of *in-situ* experiments in the COx at Bure, and (3) application at the repository scale. For heat-driven fracturing, the modeling teams started with simulating laboratory triaxial extension tests, which feature a fast-heating phase and an automatic confining control under constant vertical total stress (see Figure 3.2-1). This initial modeling was followed by THM modeling of a field experiment called CRQ, specifically designed to test the behavior of claystone exposed to a thermal fracturing stress regime (Figure 3.2-2). Modeling teams initially conducted blind predictions for the CRQ test, followed by a model comparison and improvement using CRQ data provided by Andra. For gas-pressure-driven fracturing, teams started modeling a series of benchmark exercises with increasing degrees of difficulty, followed by the simulation of several gas injection tests (PGZ) performed *in-situ* at Bure. These tests used a multi-packer system installed in two small diameter boreholes drilled in the COx, one parallel and one perpendicular to the principal stress direction (Figure 3.2-3). SFWST researchers from LBNL participated as DOE's modeling team in Task A, with a focus on the topic of thermal fracturing. See Section 6.3.3 in this report for a summary, and for more detailed information, see Section 5 of Rutqvist et al. (2024a).

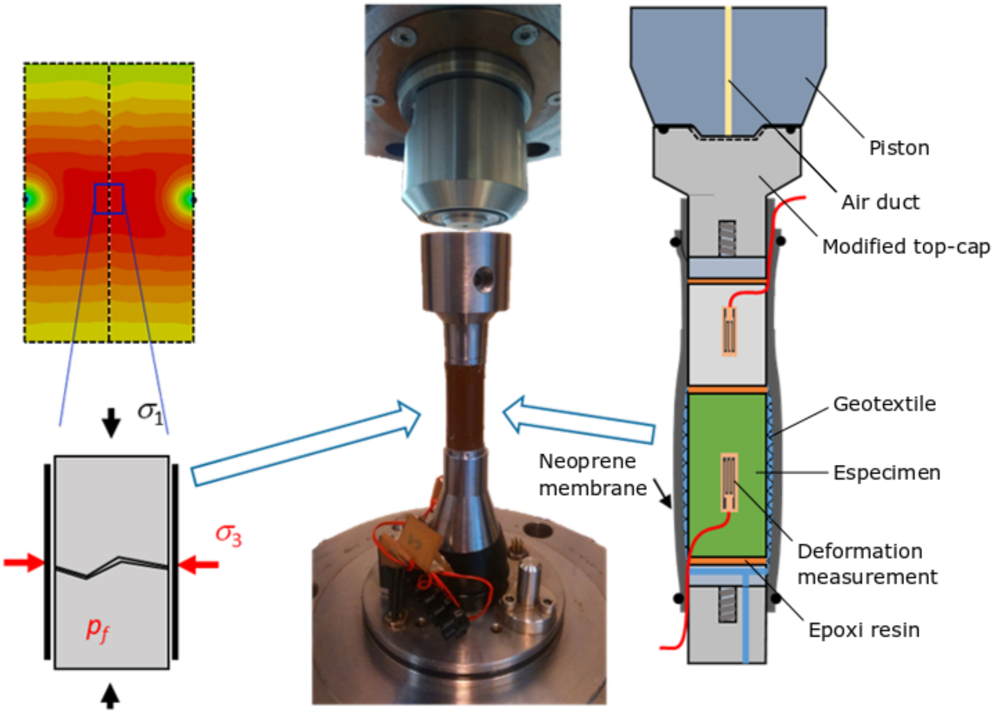


Figure 3.2-1. Schematic representation of two micro-tunnels in the HLW area with possible fracturing in the center (left) and illustration of triaxial extension experiments designed to reproduce the stress path expected in the middle between two micro-tunnels (right) (Plúa and Armand, 2020).

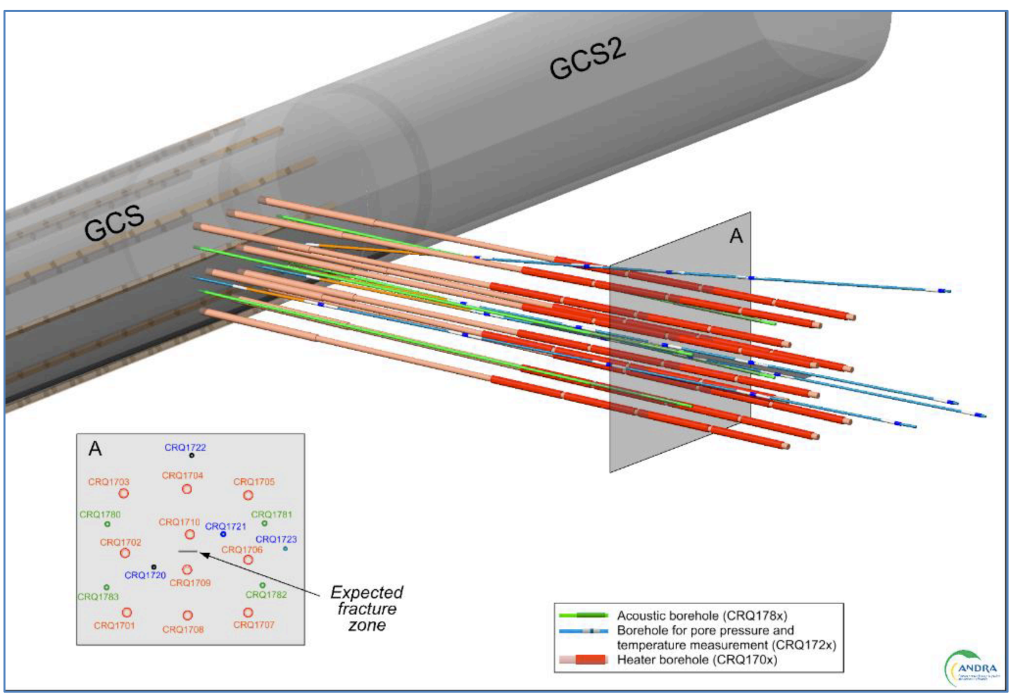


Figure 3.2-2. Borehole setup for CRQ thermal fracturing experiment (Plúa and Armand, 2020).

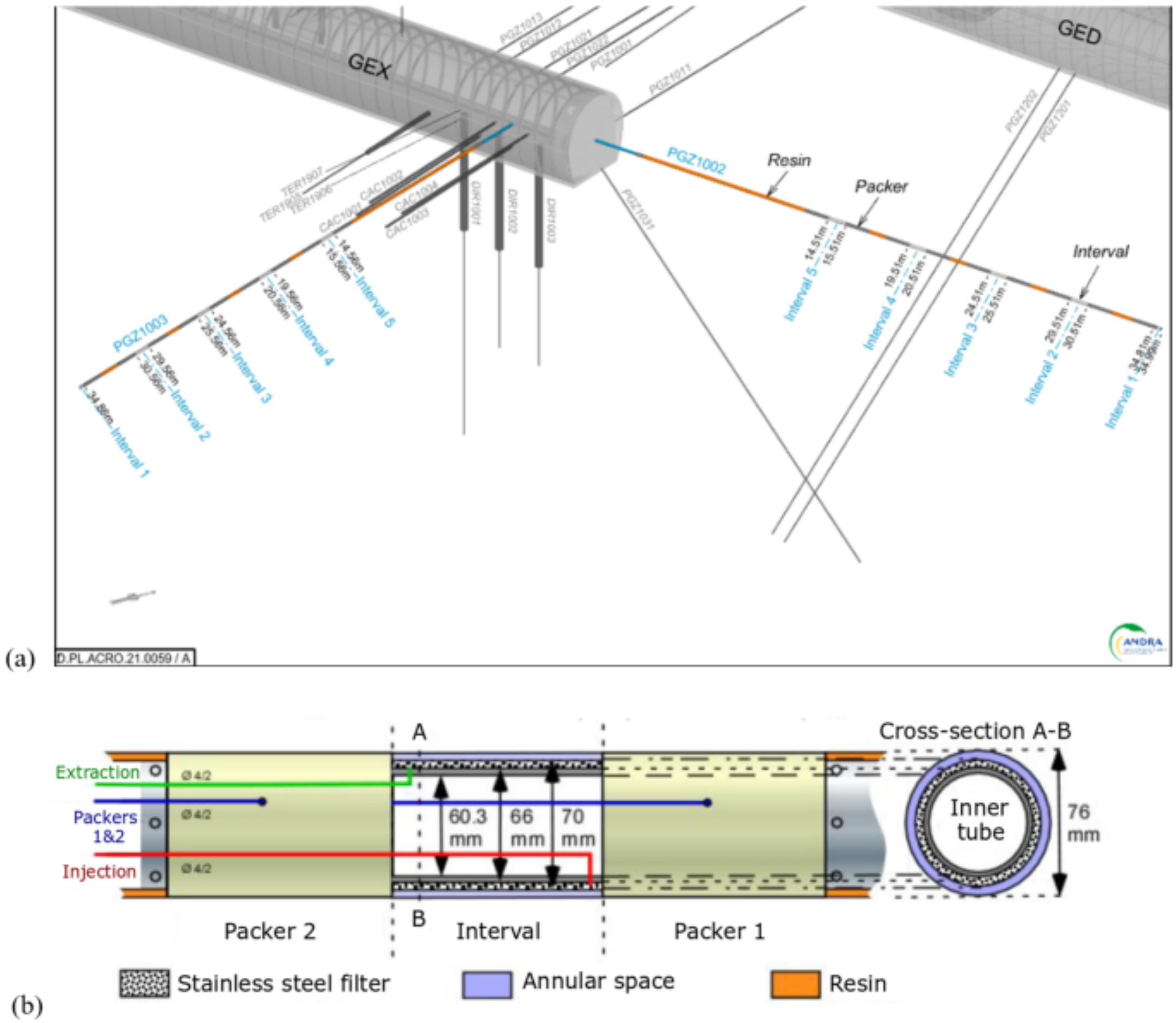


Figure 3.2-3. (a) Borehole setup for gas fracturing *in-situ* experiment (PGZ). (b) Multi-packer system for injection tests. Source: Plúa and Armand, 2020.

As summarized in the thermal fracturing synthesis paper by Plúa et al. (2024a), six research teams simulated the laboratory thermal extension tests conducted on Callovo-Oxfordian claystone (COx) samples. Then, they conducted a blind prediction of the THM response of the CRQ *in-situ* thermal hydrofracturing experiment. The teams used numerical codes with different approaches, including continuum and discrete approaches, to model these two tests. Failure criteria for their respective thermo-hydromechanical models were defined through the laboratory tests. The approaches adopted by the research teams were based on a thermo-poro-mechanical formulation, using different mechanical models: thermo-poro-elasticity (Quintessa), elasto-plasticity (BGR-UFZ and CIMNE-UPC), the phase field method (Lamcube), and weak planes modeled as Mohr-Coulomb joints, both explicitly (Ineris) and implicitly (LBNL). Among these approaches, the phase field method and the explicit joints reproduced an abrupt change in pore pressure evolution, indicating the creation of a hydraulic fracture. This was due to the coupling between the mechanical models and permeability through the damage parameter for the phase field method and through the joint opening for the explicit joints. UPC also incorporated this feature by coupling plastic deformation with permeability but obtained a homogeneous field, whereas the rest of the approaches did not include this coupling. One of the critical features of the models was the incorporation of changes in the hydraulic properties of the

COx through hydromechanical coupling. The approaches developed by the teams demonstrated their capability to analyze and reproduce fracture initiation in the COx in terms of time of occurrence and location based on their respective stress analyses. However, attempts to reproduce fracture aperture or fracture propagation were less accurate and require more work in the future.

A second synthesis paper by Plúa et al. (2024b) summarizes the comparative modeling of the gas fracturing task. Three research teams participated using three distinct simulation approaches: embedded fractures (CIMNE-UPC), damage (Lamcube), and a model combining a failure index with dilatancy-dependent permeability (BGR/UFZ). First, the research teams investigated the impact of gas migration and fluid pressurization within the Callovo-Oxfordian claystone and the fracturing threshold pressure through a series of benchmark exercises under plane strain conditions with increasing complexity. The three numerical approaches accounted for couplings between the mechanical part and hydraulic parameters, such as permeability, through different variables such as damage, fracture aperture, or equivalent plastic strain. Then, the research teams used their models to reproduce two gas injections conducted in the PGZ field test. A challenge faced by the research teams was dealing with a single study point per injection test, complicating the study of responses near the injection interval. This part included interpretative analyses with simplified approaches to understand gas pressure build-up better. Overall, the numerical simulations yielded acceptable results and provided insights into the hydromechanical response of the Callovo-Oxfordian claystone under two-phase flow conditions. Among the various features of the approaches, the coupling between mechanical and hydraulic properties played a crucial role in the *in-situ* tests. The multiple approaches adopted in gas injection applications showed promising results as they could reproduce fracture development under certain conditions. However, additional data is necessary for a better representation of fracture propagation, which fell outside the scope of Task A.

3.2.2.2 MODELING ADVECTION OF GAS IN CLAYS (MAGIC) – TASK B

This task aimed to understand the processes and mechanisms governing the advective movement of gas in compacted bentonite and natural clay-based materials, improve physics-based models of these systems, and hence support the development of performance and safety assessment models. As an extension of Task A from DECOVALEX-2019, based on laboratory data, this DECOVALEX-2023 Task B centers on the Large-Scale Gas Injection Test (LASGIT) at Äspö HRL in Sweden. After some benchmarking and blind predictions on laboratory-scale experiments, the four research teams participating in Task B were provided with field data from LASGIT. Teams then deployed the most successful modeling approaches, from laboratory-scale modeling to the field experiment with all its complexities.

LASGIT comprises a mock waste canister encapsulated in bentonite/pellets placed within a vertical deposition hole (Figure 3.2-4). The bentonite has been allowed to hydrate since 2005 after a 2-year construction phase ended with the closure of the deposition hole. Since then, gas injection tests have been conducted occasionally from several filters embedded along the surface of the canister. The test is highly instrumented: Sensors continually monitor variations in the relative humidity (RH) of the clay, the total stress and porewater pressure at the borehole wall, the temperature, any upward displacement of the lid, and the restraining forces on the rock anchors. SFWST researchers from LBNL and SNL participated as DOE's modeling teams in this gas migration task, continuing their previous work in the related DECOVALEX-2019 task. A summary of LBNL's and SNL's contributions to DECOVALEX-2023 Task B is provided in Sections 6.4.2 and 6.4.3. For more detailed information, see Section 10 of Rutqvist et al. (2024a) describing LBNL's THM modeling of the LASGIT gas injections and Section 2 of Wang and Hadgu (2024) describing SNL's development of a new theoretical model for the complex mechanism of nonlinear dynamics of gas migration.

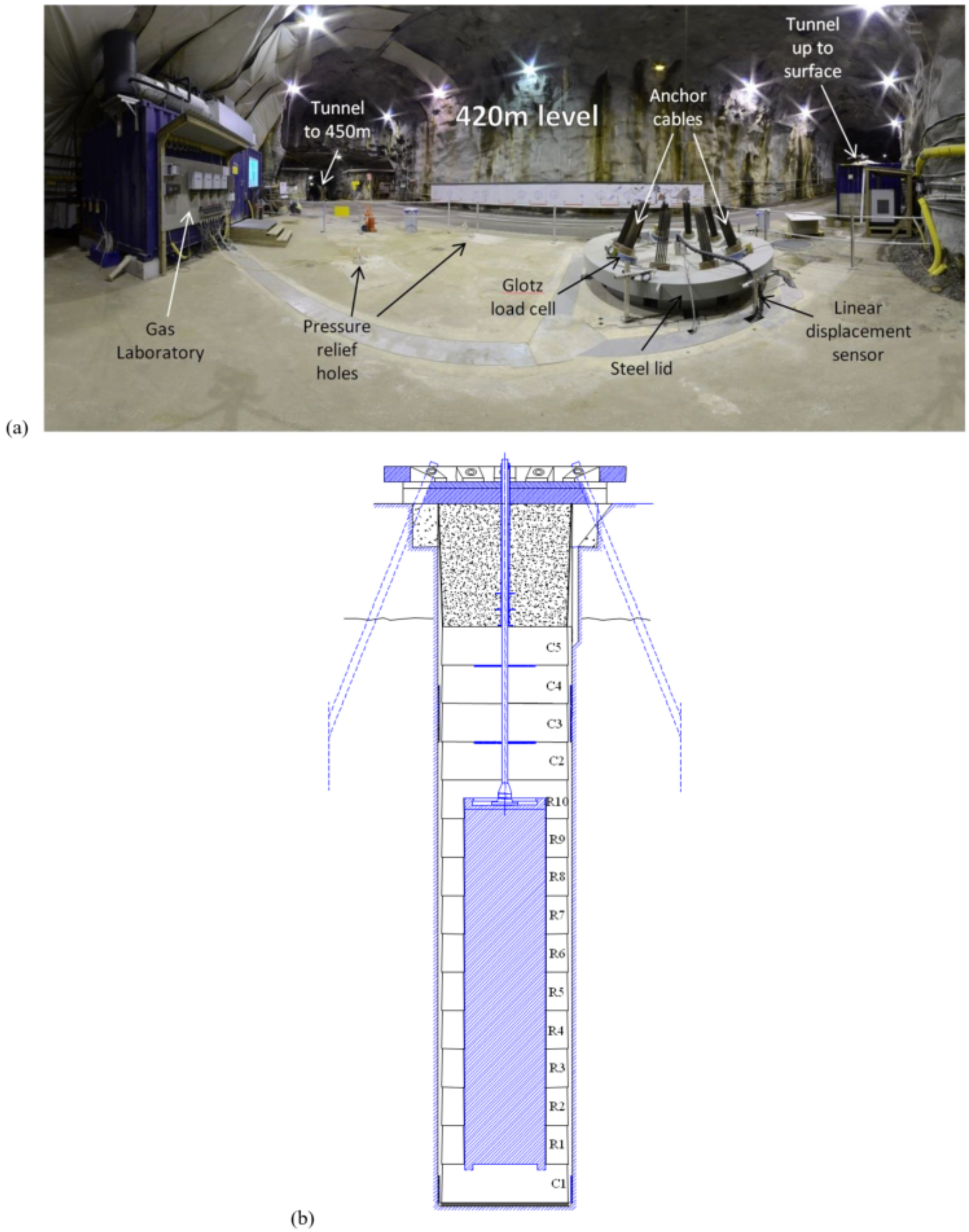


Figure 3.2-4. Large-Scale Injection Test LASGIT at Äspö HRL (Harrington and Tamayo-Mas, 2020). (a) Photo of the LASGIT installation at the 420 m level; and (b) cross-section of LASGIT setup in vertical deposition hole. There are ten filter levels R1 – R10 that have been used for segmented gas injection tests.

Collaborative modeling results for Task B are summarized in two synthesis papers: one focuses on the development of enhanced numerical representations of key processes and compares the performance of each model against high-quality laboratory test data (Tamayo-Mas et al., 2024a), and the second applies these models to the large-scale LASGIT field experiment (Tamayo-Mas et al., 2024b).

- Experimental data from the laboratory tests revealed that gas percolation in water-saturated compacted bentonite is characterized by four key features (Tamayo-Mas et al., 2024a): (i) a quiescence phase, followed by (ii) the gas breakthrough, which leads to a (iii) peak value, which is then followed by (iv) a decreasing gas flow. The research teams participating in Task B applied three models based on the multiphase flow theory, which provided good initial values and reasonable responses for gas breakthrough. Peak gas pressure values were generally reasonably well captured and could represent the negative pressure decay following peak pressure. However, other critical specific features still require a better representation. They need further improvement concerning model parameter calibration, the numerical representation of spatial heterogeneities in material properties and flow localization, and the upscaling of the related physical processes and parameters. To further understand gas flow localization, a new conceptual model was developed by one of the teams, which shows that discrete channels can which suggests that discrete channels can be induced through the instability of the gas-bentonite interface during gas injection, thus providing a new perspective for modeling gas percolation in low-permeability deformable media.
- Tamayo-Mas et al. (2024b) describe the upscaling exercise of the modeling to simulate the unique dataset from the large-scale gas injection test LASGIT performed at the Äspö Hard Rock Laboratory (Sweden). The collaborative modeling task revealed that these approaches did not need to be substantially modified to reproduce the full-scale test results. Indeed, model parameters calibrated and validated at the laboratory scale were successfully applied to predict the field scale gas flow at LASGIT, including peak gas pressure and injected cumulative gas volume. After introduction of interfaces between blocks to reflect the experimental configuration and adjustment of some parameters (e.g., higher permeability), the updated models were able to represent most of the key features observed in the experimental data, even at a large scale.

3.2.2.3 THM MODELING OF THE FE EXPERIMENT – TASK C

This task aimed to model THM processes in the Opalinus Clay host rock using data from the FE heater experiment in Mont Terri. The focus was to understand pore pressure development in the host rock and how this is affected by heating, engineering factors (e.g., shotcrete, tunnel shape), and damage due to tunnel construction and thermal effects. As described earlier in Section 3.1.2, a large dataset from the FE experiment is already available, including time series data from the tunnel's construction, tunnel ventilation, and the ongoing heating phase. The data include temperature, pore pressure, relative humidity (RH), displacement, and inclination measurement at high spatial and temporal resolution (Figure 3.2-5). The FE experiment tested engineering capabilities for construction, waste emplacement, backfilling, and the early-stage evolution of a geological disposal facility's thermal, hydraulic, mechanical, and chemical processes. This provided an opportunity to consider how the engineering of the experiment impacts the THM evolution of the system. Task C was structured into several steps, starting with a preparation and benchmarking phase (Step 0), followed by modeling of the FE heating phase (Step 1), and finally, modeling of the FE ventilation phase (Step 2) (Thatcher and Graupner, 2020). SFWST researchers from LBNL and SNL participated in this task as DOE's modeling teams. See Section 6.3.2 in this report for a summary, and for more detailed information, see Section 4 of Rutqvist et al. (2024a) and Section 2 of Hadgu et al. (2024).

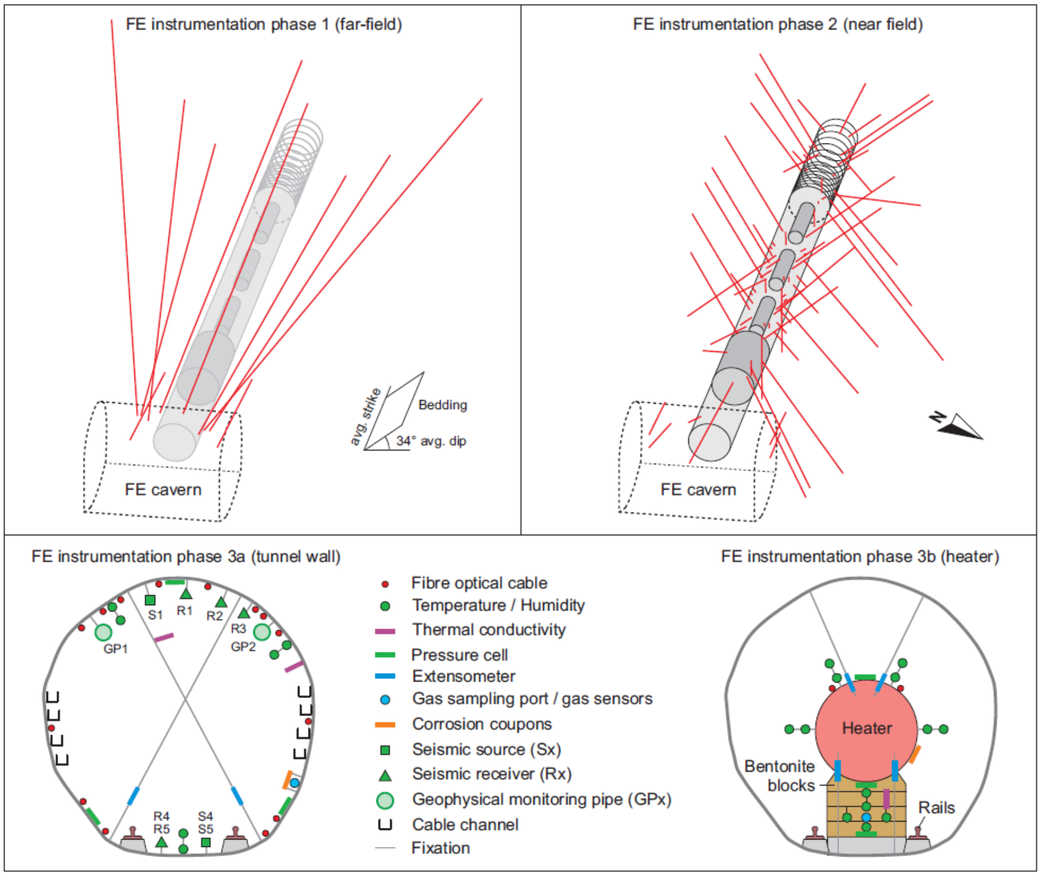


Figure 3.2-5. Diagram showing instrumented boreholes within the FE experiment and sensor locations within two cross-sections of the tunnel (Bond and Birkholzer, 2019).

As summarized in the synthesis paper by Graupner et al. (2024), ten research teams participated in the comparative modeling challenge of Task C. Based on an initial parameter set provided by the task lead, the teams started a calibration exercise in which they were free to decide which parameters they adopted for their models, whether they considered the excavation and the ventilation phase in addition to the heating phase, and if they needed to include engineering features like the shotcrete or the EDZ. Overall, the participating modeling teams were able to simulate the THM-coupled processes relevant to the FE experiment and successfully reproduced the data. Those results for the FE experiment were only achieved due to the rather extensive benchmark studies conducted beforehand. This underlines the value of well-constrained benchmarking studies when comparing complex process model implementations.

Going into more detail, the modeled results for temperature agreed very closely between the teams, especially in the sensors in the Opalinus Clay. All teams were able to reproduce the redistribution of water in the bentonite backfill due to heating. The evolution of the relative humidity showed similar trends with differences in the intensity of the dry-out effect. Modeling the pore pressure evolution was more complex because it comprises the entire interaction of the coupled THM processes. Thus, the spread between the pore pressure modeled by the teams was more significant, with some teams overestimating the pressure increase due to heating and some teams overestimating the extent of drainage. The agreement of modeled results with measurements generally improved with a larger distance to the heater. The EDZ and the shotcrete could influence the behavior of the rock, causing larger differences closer to the heater. Further research is needed to implement those influences into the models better.

Based on the calibrated models, the future evolution of temperature, relative humidity and pore pressure was predicted over the next 10 years following a change of the heat power applied in 2023 and 2024. Again, the predicted temperatures agreed very closely between the teams. Most teams did not predict an increase in relative humidity during the next 10 years after the initial dry-out.

3.2.2.4 ENGINEERED BARRIER SYSTEM EXPERIMENT AT HORONOBE URL – TASK D

The objective of this task was to better understand and be able to simulate the coupled THMC processes occurring in and around an engineered barrier system as designed in the Japanese disposal concept (see Figure 3.2-6). The Horonobe EBS experiment is a full-scale mock-up of this concept, which comprises the waste package and overpack, bentonite buffer, a mixed bentonite-soil backfill, and a low-alkaline cement plug. The heating phase of the experiment started in 2015 and ended in 2020, followed by a monitored 3-year cooling phase. Over one hundred sensors were placed in the buffer, backfill, and the surrounding rock mass during the installation of the experiment to monitor the coupled THMC processes, including temperature, total pressure and pore pressure, water content, resistivity, displacement, and strain (Figure 3.2-7). JAEA designed two main modeling steps for this task: Step 1 involved modeling several laboratory tests, and Step 2 featured the full-scale EBS heater experiment (Sugita, 2020). SFWST researchers from SNL participated as DOE's modeling team in this task. See Section 6.1.4 in this report for a short summary, and for more detailed information see Sections 2-3 of Jové-Colón and Lopez (2024). Note that JAEA plans to dismantle the *in-situ* experiment 2026- 2027, followed by detailed characterization of EBS and host rock samples. This will allow for an ultimate confirmation of the THM predictions conducted within this modeling task.

Six research teams performed the TH or THM (depended on research team approach) numerical analyses of Task D using a variety of computer codes, formulations and constitutive laws. Some joint lessons learned are briefly summarized below (see also the synthesis paper by Sugita et al., 2024):

- The stepwise approach of Step 1 (laboratory tests) preceding Step 2 (*in-situ* test) turned out to be successful in that it allowed reasonable prediction of the EBS heater experiment. In the case of parameters which are difficult to derive through direct laboratory experiments, the choice of these parameters can significantly impact the modeling predictions of the *in-situ* experiment (e.g., relative gas permeability). The task lead concluded that it is important to obtain such parameters through appropriate indirect methods (i.e., experiments + parameter identification techniques), before the simulation work of the *in-situ* experiment can be tackled.
- The application of an elasto-plastic constitutive model for the mechanical processes in the buffer material improved the reproducibility of the swelling behavior of the buffer material. When an elastic constitutive model is applied, adding an equation for considering swelling displacement can also simulate the measured deformation well.
- 3D simulation of the EBS experiment was difficult for some teams due to the computational demand imposed by the constitutive equations, which increased simulation times drastically. As a result, some research teams instead used 2D axisymmetric or 2D plane strain models. Simplified 2D representations of the system can be adequate but requires careful assumptions to produce output that is directly comparable to the data.

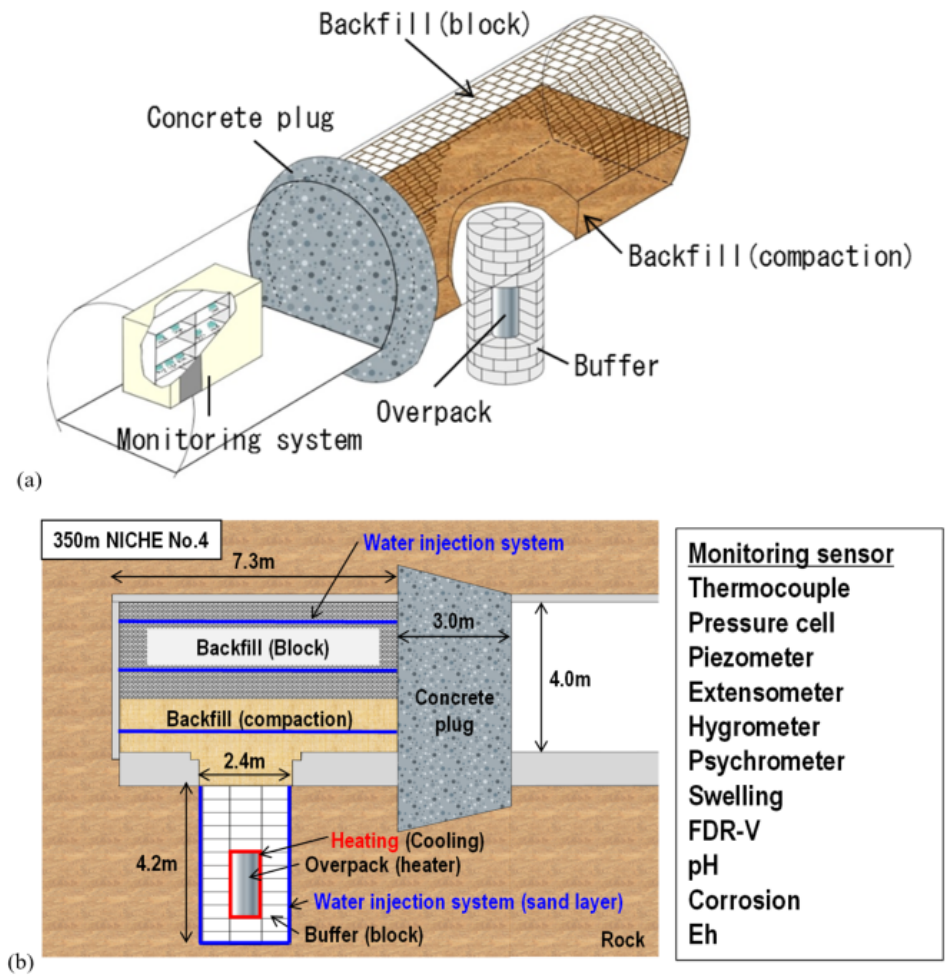


Figure 3.2-6. Schematic view of the Horonobe full-scale *in-situ* EBS experiment (Bond and Birkholzer, 2019). (a) 3D setup and (b) cross-section.

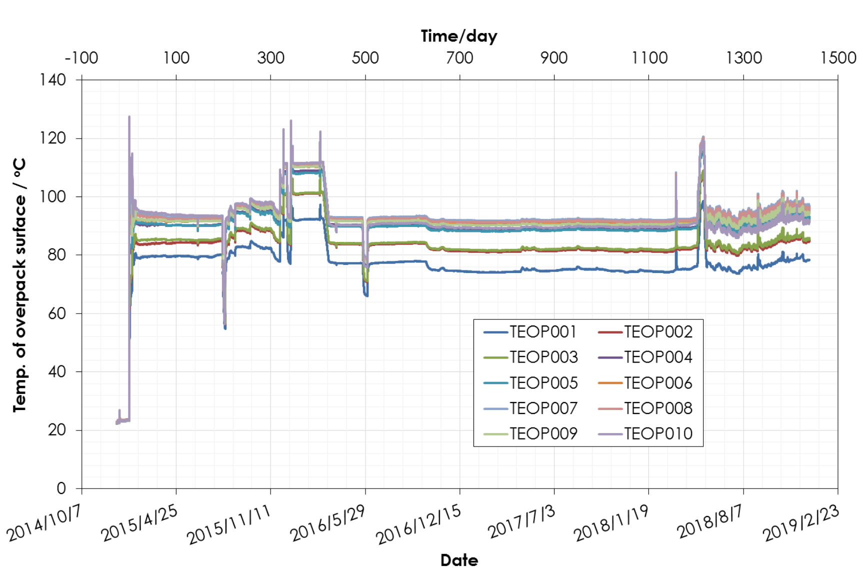


Figure 3.2-7. Temperature evolution in the EBS experiment (Sugita, 2020).

3.2.2.5 BRINE AVAILABILITY IN SALT (BATS) – TASK E

The objectives of this task were to observe and predict the coupled processes governing water availability to heated excavations in geologic salt. Brine availability strongly impacts the long-term performance of salt repositories for heat-generating radioactive waste. Brine leads to the corrosion of waste forms and packages and the possible dissolution of radionuclides, with brine transport being a potential transport vector to the accessible environment.

The task utilizes data from the BATS tests conducted at WIPP to (1) confirm the strengths and types of coupled THMC processes (i.e., thermal, hydrologic, mechanical, and chemical – THMC) that govern preferential brine flow paths and canister corrosion (e.g., Figure 3.2-8), and (2) develop and validate numerical and constitutive models for coupled processes and salt migration in bedded salt.

The BATS field tests used in DECOVALEX-2023 were conducted between 2018 and 2021 in short horizontal boreholes at the repository level (~650 m depth) in the US Department of Energy's Waste Isolation Pilot Plant (WIPP) (Kuhlman et al., 2021a,b):

- A preliminary "shakedown" test was performed in the summer of 2018 to compare heater designs and test equipment in the salt environment, completed in boreholes cored in 2013 (BATS "1s"). Brine inflow was quantified by circulating dry N_2 gas behind a packer and through desiccant (i.e., grams of water per day). Temperature data (thermocouples) were collected during several sequential multi-day heating episodes at different heater power levels. These results provide the first dataset to test numerical modeling approaches.
- A second test series was conducted from January to March 2020 (Phase 1a), in two parallel and nearly identical test arrays drilled specifically for BATS, one heated with a source borehole maintained at ~96°C (2 weeks pre-heating data, 1 month of heated data, 2 weeks cool-down data) (Figure 3.2-9), the other unheated. The tests provided data on the volumetric flow rate and composition of fluids (e.g., brine and steam) and tracers entering the boreholes through time. Geophysical data (i.e., electrical resistivity tomography (ERT), acoustic emissions, ultrasonic wave velocity, temperature, fiber-optic distributed temperature, and strain) complement solid (i.e., cores around seals and heaters before and after testing), liquid (i.e., samples of brine with natural and added tracers), and gas (i.e., stable water isotopes and gas chemical composition) sampling (Figure 3.2-10). Fluid samples and geophysical data have been collected before, during, and after the heating phases.
- BATS Phases 1b and 1c were conducted between January 2021 and May 2021. This third test series involved the addition of gas (1b) and liquid (1c) tracers in the same heated and unheated boreholes of the BATS Phase 1a location.

The task lead for Task E, Kris Kuhlman from SNL, developed a task structure and schedule that started with simplified benchmarks and then progressed to more complex field test modeling. Short descriptions of the three steps are given below:

- **Step 0 - Simple single process H and T benchmarks**: Relatively simple simulations, either synthetic or well-constrained experiments, to act as a 'warm-up' for participants and allow codes and process models to be compared,
- **Step 1 - Coupled processes benchmarks**: More complex benchmarks involving TH and THM processes in salt, with single and multi-phase flow,
- **Step 2 - Heated Brine inflow test cases**: More complex modeling with THM multi-phase flow coupling, with detailed comparisons against field experimental data. The test cases include some historic data sets from past experiments as well as the BATS measurements.

For SFWST, a joint modeling team was formed to participate in Task E, consisting of the national labs conducting, analyzing, and modeling the BATS test (SNL, LANL, LBNL). See Section 6.6.3 in this report for a short summary of SFWST's BATS modeling, and for detailed information see Section 5 of Rutqvist et al. (2024b), Section 3 of Mills et al. (2024), and Section 2 of Guiltinan et al. (2023).

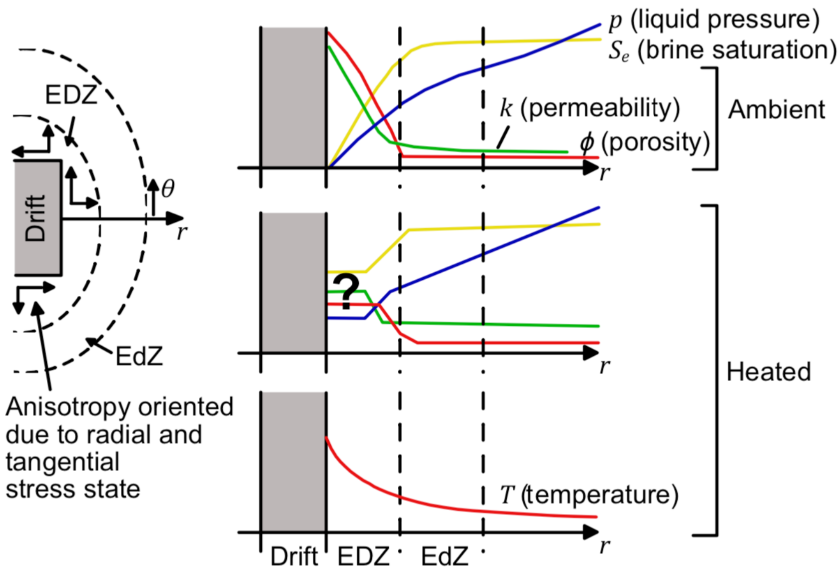


Figure 3.2-8. Schematic trends in hydrological properties and state variables from a drift in salt to the far field under ambient (top) and heated (bottom) conditions (Kuhlman, 2020).

Figure 3.2-9. BATS heated array (Kuhlman, 2020).

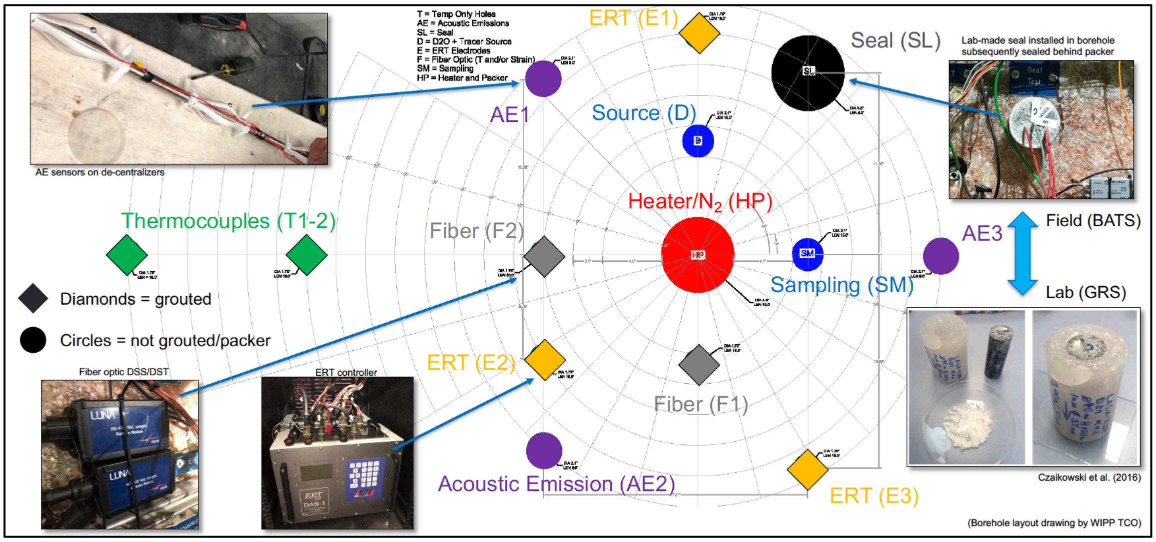


Figure 3.2-10. Borehole layout with a central heater borehole and satellite monitoring boreholes in a vertical cross-section perpendicular to the heater element (Kuhlman, 2020).

In general, the collective modeling of brine inflow conducted by teams from the U.S., United Kingdom, and Germany led to an increased understanding of the complex processes expected to occur in the EDZ of a salt repository for the disposal of heat-generating radioactive waste (see synthesis paper by Kuhlman et al., 2024a). In the longer term (tens to hundreds of years), The drift and the damage (i.e., ϕ and k) of the EDZ will creep shut, and the dynamic processes observed in BATS will be less critical. Understanding these early-time and short-distance processes is essential to quantify the initial conditions that performance assessment models will need, including the effects of model initialization and the amount of brine expected to flow into the drifts, as radionuclides dissolved in brine would typically be the primary release pathway. Understanding processes going on in the near field and short term is also crucial if any future repository design is to be optimized.

There were a range of approaches from the teams, from mechanistic to prescriptive. Given the uncertainties in the problem, some teams used one- or two-dimensional models of the processes, while others included more geometrical complexity in three-dimensional models. As the Task Lead Kris Kuhlman pointed out, the discussions between the task lead and the teams were a critical part of the learning as a group (i.e., between the teams), as different approaches were attempted, modified, and sometimes dropped. The primary Task E lessons learned were the impact of hydrologic initialization methods (wetting up vs. drying down), the difference between confined and unconfined thermal expansion, and the significant changes in permeability associated with heating and cooling.

The benefits from the Task E exercise extend beyond the improved conceptual understanding derived from modeling and the interactions between the teams; they also extend to the experiment design and execution. The second phase of BATS is already underway (referred to as BATS2), and the field test has been collecting additional data to use in the current phase of DECOVALEX-2027 (Section 3.2.3.3).

3.2.2.6 PERFORMANCE ASSESSMENT (PA) – TASK F

The ultimate objective of this DOE-led task was to build confidence in the models, methods, and software used for PA, or safety assessment, of deep geologic repositories and/or to bring to the fore additional research and development needed to improve PA methodologies. To achieve this objective, Task F involved a staged comparison of models and methods used in different PA frameworks, including (1) coupled-process submodels (e.g., waste package corrosion, spent fuel dissolution, radionuclide transport, etc.) comprising the full PA model, (2) deterministic simulation(s) of the entire PA model for defined reference scenario(s), (3) probabilistic simulations of the entire PA model, and (4) uncertainty quantification (UQ) and sensitivity analysis (SA) methods/results for probabilistic simulations of defined reference scenario(s). The task focused on performance measures indicative of the ability of the repository system to isolate radionuclides from the biosphere through containment and retardation. Performance measures were related to (1) the overall performance of the repository system, such as radionuclide concentrations in groundwater some distance from the repository, and (2) the performance of individual components of the engineered or natural system, radionuclide flux from one component of the system to another. Before DECOVALEX-2023, SFWST had developed a suite of reference cases to conduct 3D probabilistic performance simulations of generic repositories in various host rocks (Figure 3.2-11). The DOE crystalline and salt reference cases were valuable starting points for defining Task F.

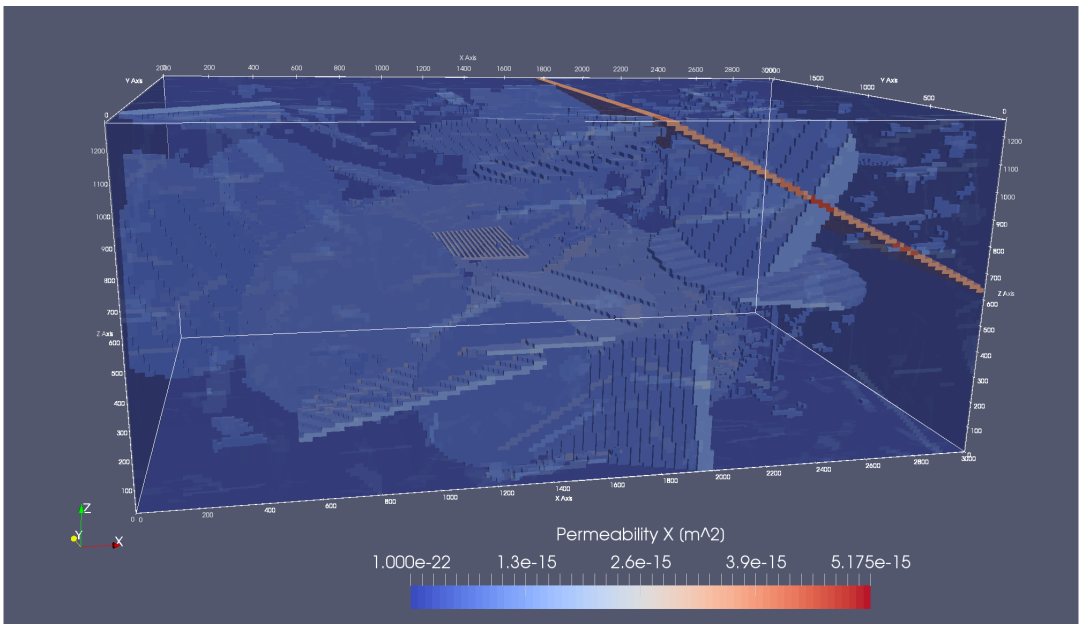


Figure 3.2-11. Generic reference case for a crystalline repository as developed by the SFWST campaign. The figure shows emplacement 3,360 waste packages in 168 drifts placed 20 m apart, with a fracture network based on Forsmark (Sweden) fracturing characteristics (Stein, 2020).

Task F investigated two generic reference cases in parallel: a repository for commercial SNF in a fractured crystalline host rock (Task F1) and a repository for commercial SNF in a salt formation (Task F2) (Stein et al., 2020). Teams could choose to participate in either one or both reference cases. Although a direct comparison cannot be made between simulations of a crystalline repository and simulations of a salt repository, lessons learned regarding, for instance, methods of coupling process models, propagating uncertainty, or conducting sensitivity analysis were found be transferable between concepts. Emily Stein from SNL served as task lead for the first 2 years; Paul Mariner later replaced her for the crystalline case and Tara LaForce for the salt case. See Section 6.9.2 in this report for a summary of SNL's contributions to these tasks, and for more detailed information, see Mariner et al. (2024b) and LaForce et al. (2024b). Note that the comparison of performance assessment approaches continues in the current DECOVALEX-2027 phase (see Section 3.2.3.8), with an enhanced focus on sensitivity analysis and uncertainty quantification.

The crystalline case (F1) moved from a benchmarking phase, involving, for example, flow in simple fracture geometries and more complex modeling challenges with stochastic fracture networks and transport processes, to comparative modeling of the large-scale reference case for a mined repository in fractured crystalline rock. The eight research teams in Task F1 experimented with alternative modeling approaches, such as discrete fracture network (DFN) models versus equivalent continuous porous medium (EPCM) models.

- In a synthesis paper focusing on the benchmarking phase, Mariner et al. (2024a) described the three benchmark problems as follows: 1) a pulse of a conservative tracer into a network of four intersecting deterministic fractures, 2) a pulse of a set of tracers into the same domain but with the addition of 1,089 stochastically generated fractures, and 3) a continuous point source of the same set of tracers into the same domain with the stochastic fractures. To study the effects of model approaches on flow and transport, all teams share the same fracture network realization. Excellent agreement in breakthrough behavior was observed for all models to at least the 75th percentile. At the 90th percentile, breakthrough results showed more significant differences between modeling teams, indicating that several models retain substantially higher fractions of tracer in regions of slower-moving water. Breakthrough curves were further evaluated using moment analysis. Large deviations in the first moments prompted several discoveries, including numerical errors caused by coarse meshing at fracture intersections and mistakes in the retardation of a sorbing tracer. Overall, the lessons learnt and verification afforded by the developed benchmark models provide valuable information about choices when modeling flow and transport in fractured rock.
- In a second synthesis paper for Task F1, Leone et al. (2024) describe the collaborative modeling results for a mined repository's large-scale generic reference case in fractured crystalline rock. The reference case is a simplified version of a performance assessment focused on transporting two conservative tracers from the deposition hole to the surface, neglecting waste package performance. Quantities of Interest (QOI) were compared, such as remaining tracers in the repository and fluxes across the domain. Technical and time constraints led some teams to exclude parts of the engineered barrier system, resulting in faster release of tracers and radionuclides from the repository region. Comparing all models highlighted the importance of explicitly including drifts, buffers, and backfill in the reference case models. There were still some differences in model results for the models with comparable repository geometry and inventory evolution. The main differences between these models were in how to represent the fracture network and simulate transport of the two tracers. Overall, the results indicate the sizeable effects of model uncertainty and demonstrate the utility of various approaches to build confidence in a performance assessment.

The salt reference case (F2) started with a detailed discussion about the features and characteristics of a salt reference case that is relevant to all participating teams and creates critical performance assessment challenges. The five research teams participating in Task F2 then developed and simulated the modeling scenario of a salt dome repository with a shaft seal failure scenario (see synthesis paper by LaForce et al., 2024). The teams made many model assumptions, ranging from compartmentalized networks to full 3D models of the salt formation and repository. Despite differences in the modeling strategies, all models indicate that salt compaction and diffusion of radionuclides in brine are key processes in the repository. For the isothermal spent nuclear fuel and vitrified waste scenario with multiple early failures considered, all models indicate little of the disposed radionuclides will migrate beyond the repository seal over the 100,000-year simulations. Generally, the model output quantities have the most significant differences over the short term and near the waste. Disparities between the models are believed to be due to differing simplifications from the conceptual model.

3.2.2.7 SAFETY IMPLICATIONS OF FLUID FLOW, SHEAR, THERMAL, AND REACTION PROCESSES WITHIN CRYSTALLINE ROCK FRACTURE NETWORKS (SAFENET) – TASK G

Understanding of shear reactivation of pre-existing discontinuities for brittle host rocks is an area of considerable interest for radioactive waste disposal. The potential for existing features to undergo shear displacements and related changes in permeability as the result of coupled thermal, mechanical, hydrological, and chemical effects can have significant impacts on repository safety functions (e.g., creating permeable pathways or, for substantial displacements, mechanical damage of waste packages). The purpose of this task was to improve our quantitative understanding of fracturing processes in brittle rocks caused by mechanical (shear), hydraulic (fluid injection), and thermal (heating) processes via the following task activities related to core-scale laboratory experiments (Figures 3.2-12 and 3.2-13):

- Evaluation of mechanical (M) laboratory test results derived from constant normal load (CNL) direct shear tests and constant normal stiffness (CNS) direct shear tests as well as high-resolution fracture surface scans (TU BA Freiberg) (Step 1). This step elucidated the mechanics of rough fractures and how they were affected by shear and normal displacement.
- Investigation of HM results obtained with the GREAT cell (University of Edinburgh) with a focus on fundamental shear processes under complex 3D stress states in large samples (200 mm diameter and height) (Step 2). Building on Step 1 and using the same rock samples, this step elucidated controls on fracture fluid flow under repository *in-situ* conditions, focusing on deformation, fracture normal stress, shear stress, and fluid pressure.
- Investigation of TM results obtained from tri-axial tests conducted at the Korea Institute of Civil Engineering and Building Technology (KICT) in the Republic of Korea focuses on shear processes triggered by thermal stresses (Step 3). These laboratory experiments were conducted at a 1.1 Meganewton load capacity in each axis and 150°C temperature. Building on Steps 2 and 3, this step answered the following key scientific question: Can long-term heating effects induce the shear slip of a stressed fracture, and if so, what factors predominantly influence the shear slip process?
- Evaluation of impacts of fully coupled THM processes. This optional step was not achieved during the DECOVALEX-2023 timeline.

The focus of this task was to explore the link between micro-scale THMC effects acting on fracture surfaces and asperity contacts with emergent fracture properties such as permeability. The experiments were conducted on representative granite samples with pre-existing, well-characterized discontinuities. This task was novel for DECOVALEX because it focused on understanding fundamental processes, based in part on previous DECOVALEX work, but also attempted to link these processes to key safety performance functions in radioactive waste disposal facilities. The wide range of high-quality experiments and conditions being examined allowed process understanding to be developed and robustly tested using state-of-the-art approaches.

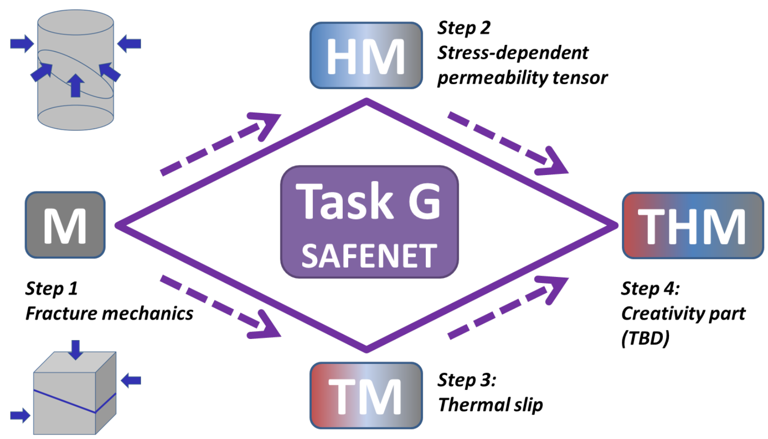


Figure 3.2-12. Task G structure (Kolditz et al., 2020).

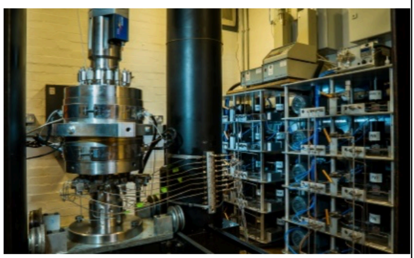
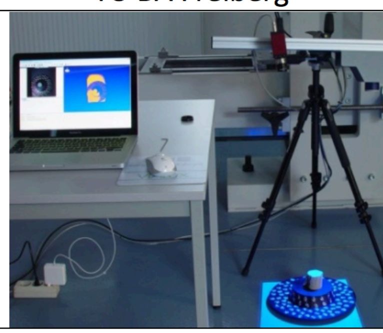
Experimental Facilities		
University of Edinburgh	TU BA Freiberg	KICT
		
GREAT cell for polyaxial (including true-triaxial) THMC testing	3D surface and body scanner (max. 30µm resolution)	True-triaxial THM testing, High-resolution X-ray µCT, AE monitoring system

Figure 3.2-13. Experimental facilities used in this task (Kolditz et al., 2020).

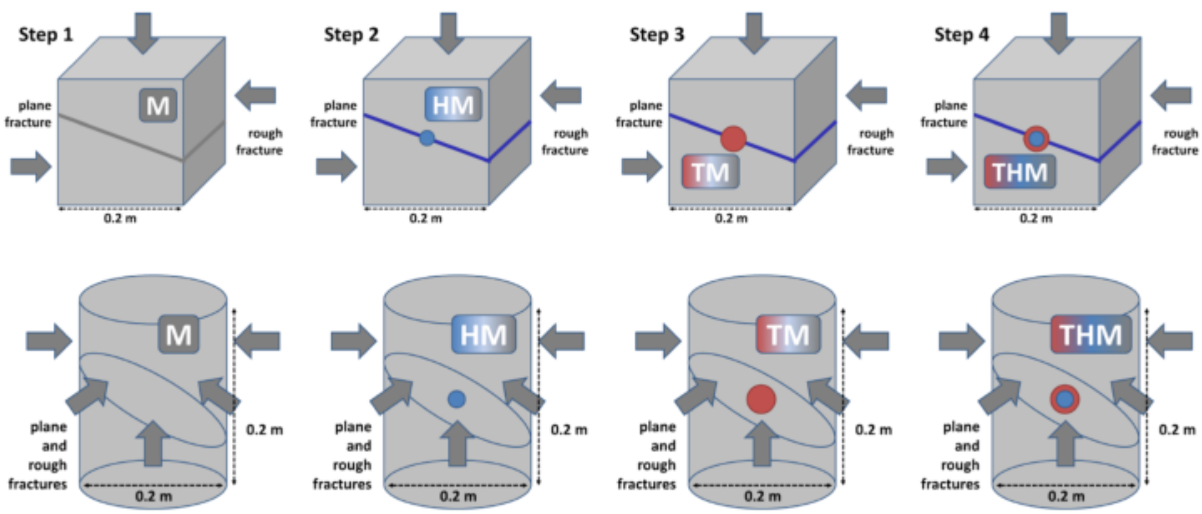


Figure 3.2-14. Task G benchmarking ideas (Kolditz et al., 2020).

Task participants from multiple international modeling groups started with benchmark simulations to set the stage for more complex blind-prediction modeling of laboratory experiments. For example, one of the first benchmarks investigated the mechanical behavior of rough fractures before and after mechanical shear. Shearing of a single fracture in a rectangular domain exposed to a differential (shear) load was simulated, and the results were compared with an analytical solution. Modeling teams subsequently moved on to the experimental tasks in Step 1 (TU BA Freiberg test), Step 2 (GREAT cell tests), and Step 3 (KICT tests). These steps were handled in parallel, and not all teams participated in each step. SFWST researchers focused on Step 2 and Step 3: SNL scientists applied the COMSOL Multiphysics™ software to interpret the experimental data from the GREAT cell. LBNL scientists applied FLAC3D to analyze the experiments of thermal slips of single fractures that were conducted at KICT. See Sections 6.5.2 and 6.5.3 in this report for summaries, and for more detailed information, see Section 1 in Wang and Hadgu (2024) and Section 5 in Hu et al. (2024).

As summarized in the synthesis paper by Kolditz et al. (2024), eight international modeling teams collaborated to simulate and predict the HM and hydro-thermal response of fractured rock exposed to M, HM, and TM perturbations. The teams used a variety of different numerical methods and computing packages. They applied sharp fracture approaches (such as xFEM) and diffuse fracture approaches (phase-field models) for fracture mechanics. In particular, the research teams developed and applied various constitutive models for fracture behavior and improved fundamental physical understanding of these complex processes. Modeling analysis of Step 1, Step 2, and Step 3 experiments showed that, based on the developed methodology and verification of numerical tools in a cross-referenced fashion, novel HM and TM experiments results could be better understood and reproduced numerically with sufficient accuracy representing the primary process characteristics.

- The Step 1 Freiberg experiments underpinned that fracture roughness plays a crucial role in rock matrix damage and fracture propagation, affecting stress-dependent permeabilities. Joint roughness coefficients (JRC) and joint compressive strength (JCS) are important parameters for these processes. According to experimental observations, damage occurred not only to the fracture asperities but also propagated into the rock matrix in the form of microcracks and localized macrocracks.
- The Step 2 GREAT cell experiments analyzed in Step 2 were the first to collect precise HM data for strains in variable polyaxial stress fields and to determine the stress-dependent fracture permeabilities using the corresponding models. This improved the understanding of permeability changes during stress redistributions, e.g., excavating cavities in the crystalline basement.
- The Step 3 KICT experiments, and corresponding TM modeling, have shown under which conditions thermal shearing can occur, i.e., when thermal effects influence mechanical shear strength.

The influence of the coupled processes could be precisely quantified by systematically investigating the mechanical and then the hydro-and thermo-mechanical processes in the Freiberg, GREAT cell, and KICT experiments. Additional work is needed to enhance modeling capabilities for coupled microscale THM fracturing processes, which was not accomplished in the DECOVALEX-2023 phase. Furthermore, there is a need to comprehend fracture processes across different scales. These remaining challenges are part of the current DECOVALEX-2027 task described in Section 3.2.3.1.

3.2.3 DECOVALEX-2027

The current DECOVALEX-2027 phase started in Spring 2024 and will end in late 2027. The project organized several planning sessions during workshops in 2022 and 2023 to identify suitable tasks for this phase. At the end of this process, prospective funding organizations decided on eight exciting tasks to be included in DECOVALEX-2027. A total of 18 funding organizations is participating in DECOVALEX-2027, one more than in the previous phase. Most funding organizations from DECOVALEX-2027 continued into the current phase, but JAEA dropped out. At the same time, the Korean Institute of Geoscience and Mineral Resources (KIGAM) and the German DynaFrax joined as new partners. Jens Birkholzer from LBNL continues to serve as the Chair of the DECOVALEX initiative. The eight modeling tasks envisioned for DECOVALEX-2027 are listed in Table 3.2-4; more information on each task is given in Sections 3.2.3.1 through 3.2.3.8. The table nicely shows how the DECOVALEX-2027 tasks span various modeling challenges, starting with fundamental process understanding, sealing systems, fractured rock characterization, and system-scale modeling. SFWST scientists serve as task leads for two tasks, namely BATS2 and the Repository Modeling and Performance Assessment tasks, and they are involved in all but one of the eight tasks (with the participation of LBNL, SNL, and LANL scientists).

Table 3.2-4. Proposed modeling tasks for DECOVALEX-2023 (Birkholzer and Bond, 2023).

Understanding of Processes and Impact on Safety in Different Host Rocks
• SAFENET-2: THM Fracture Mechanics in Crystalline Rocks - From Lab to Field Scale
• HyMAR - Hydro-Micromechanics of Argillaceous Rocks
• BATS2 (Brine Availability Test in Salt – Phase 2)
Sealing Systems
• SANDWICH - HM Interactions Between the Host Rock and Novel Shaft Seals
• BaSiSS - Bentonite and Sand in Sealing Systems
Fractured Rock Characterization: Using Pilot Hole Data and Repository Construction Data
• FRESCIP - Fractured Rock Extrapolation, Suitability Criteria and Inflow Prediction
System-Scale Modeling and Performance Assessment Methodologies
• ANALOG - Multiscale Long-term Radionuclide Transport at Cigar Lake Uranium Ore Body
• Repository Modeling and Performance Assessment for Two Generic Repository Cases

3.2.3.1 SAFENET-2: THM FRACTURE MECHANICS – FROM LAB TO FIELD SCALE

This task aims to better understand fracture nucleation and evolution processes in crystalline rocks, with applications in nuclear waste management and geothermal reservoir engineering. This task is led by the Helmholtz Centre for Environmental Research, the University of Edinburgh, and DynaFrax. Teams collaborate to improve models for these geosystems, which has implications for performance and safety assessment and reservoir optimization. As a continuation of the DECOVALEX-2023 SAFENET task, with its previous focus on benchmarking fracture models and experimental laboratory analyses (Section 3.2.2.7), SAFENET-2 is dedicated to model extension and validation from the laboratory to the field scale. Field-scale studies will initially focus on the crystalline rock systems at the Teaching and Research Mine URL Reiche Zeche, located in Freiberg granite in Germany (Figure 3.2-15). At a later stage, the activities may be extended to the currently planned geothermal URL (GeoLaB) in hydrothermally altered crystalline rocks in the Upper Rhine Valley in Germany. Construction of GeoLaB will start in 2025. Therefore, core samples from GeoLaB for laboratory experiments should be available in the later phase of DECOVALEX-2027.

Experimental datasets available to participants will first come from a unique set of HM and THM laboratory experiments that allow for polyaxial testing of fractured rock samples (GREAT cell, polyaxial THM cell). In addition, KICT plans an advanced experiment of thermally induced slip of natural rock joints representing a small mock-up of the Swedish disposal system. The thermally induced fracture slip and propagation under a true triaxial stress state will be characterized by acoustic emission monitoring, X-ray computed tomography (XCT) scanning, and high-resolution laser scanning. The experimental basis at the field scale is provided by the STIMTEC experiment in the URL Reiche Zeche, where stimulation tests with periodic pumping tests and high-resolution seismic monitoring have been conducted (Boese et al., 2021; 2022; Martínez et al., 2021). Together with the laboratory experimental data, the STIMTEC experiment will provide a basis for upscaling fracture models from lab to field scale concerning HM-induced fracture processes.

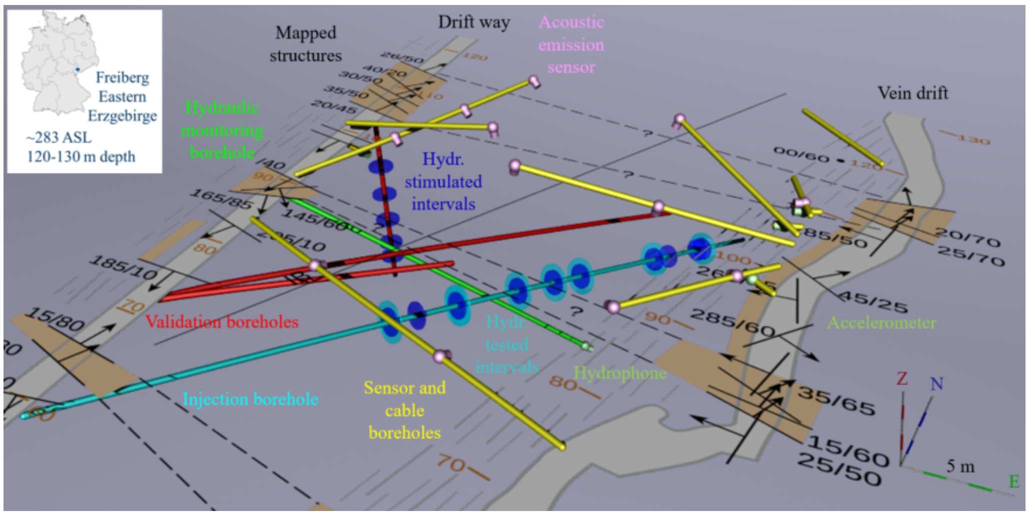


Figure 3.2-15. Schematic of STIMTEC stimulation experiment (Kolditz, 2023).

Figure 3.2-16 provides a schematic of the structured work plan for this task. Based on increasing levels of complexity from lab to field scale, an incremental approach to developing this task is proposed.

- **Step 1**: Simulation of lab scale HM fracture propagation experiments (3D bench scale hydraulic fracture under polyaxial stress experiments with fiber optic strain measurements),
- **Step 2**: Simulation of field scale HM and coupled seismicity (fluid injection into rock mass and measurement of seismicity, URL Reiche Zeche),
- **Step 3**: Methodology, computer, and data science: THM fracture mechanics (including the analysis of KICT lab experiments), interactive and collaborative benchmarking, ML, and
- **Step 4**: Synthesizing the knowledge concerning upscaling of fracture models from lab to field scale for PA/SA of waste disposal concepts in crystalline host rocks. Knowledge transfer to related geoenergy applications (i.e., enhanced geothermal systems in crystalline reservoir rocks).

As DOE's modeling teams, the SFWST researchers from LBNL and SNL are participating in this task, continuing the related DECOVALEX-2023 task.

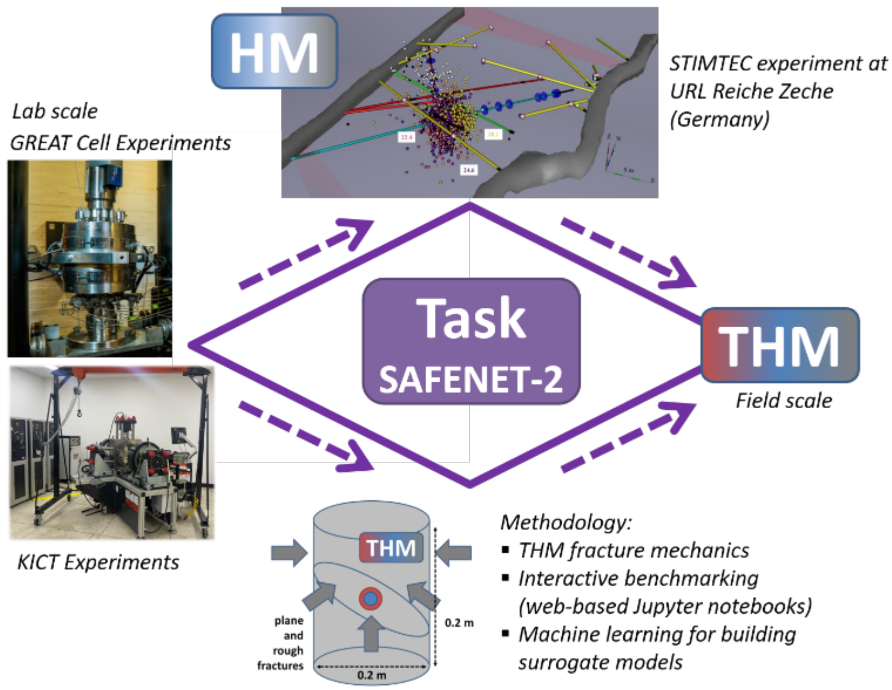


Figure 3.2-16. Task B structure (Birkholzer and Bond, 2023).

3.2.3.2 HYMAR – HYDRO-MICROMECHANICS OF ARGILLACEOUS ROCKS

The main objective of HyMAR is to understand better the processes and mechanisms at the microscale that govern the damage/deformation/dilatancy behavior of argillaceous rocks and the influence of this behavior on gas and water migration at relevant repository scales. This task is led by the Canadian regulator CNSC, the German BGR, and the British Geological Survey (BGS). The task is motivated by recognizing that the geosphere is the significant barrier to radionuclide migration in argillaceous rocks. The movement of groundwater and gas that transport the radionuclides strongly depends on the host rock's deformational/damage evolution. This evolution needs to be evaluated, necessitating the development of robust constitutive models to simulate the mechanical damage-failure behavior of the rock. Constitutive models are mainly based on macroscopic observations that need to be complemented with observations at the microscale to validate the model assumptions. Constitutive models developed from laboratory tests must also be validated with *in-situ* large-scale experiments to be used with confidence in PA/SA of deep geological repositories in the same type of rock.

To achieve this goal, HyMAR provides experimental data and pursues modeling at three different scales as follows: (1) Laboratory consolidated-undrained (CU) triaxial tests provide microscopic observations of damage and dilatancy, (2) Gas injection tests on Opalinus clay conducted at bench-scale provide understanding of gas migration at meso-scale, and (3) *In-situ* tests at Mont Terri URL such as the Gas Injection (GT) Experiment provide data at relevant macroscopic scales. The GT experiment, described in Section 3.1.5.2, is currently underway and will last for another year or so (Figure 3.2-17).

An incremental approach to the development of this task is proposed as follows:

- **Step 1** Focuses on developing constitutive models and their calibration with CU triaxial tests in conjunction with microscopic observation of damage/microfracturing. The models should be able to predict the evolution of pore pressure, the onset of dilatancy, strain localization, and shear banding, and the influence of bedding orientation,

- **Step 2**: Consists of implementing the constitutive models developed in Step 1 to simulate gas injection in Opalinus Clay samples (at two different bedding orientations) at the bench scale,
- **Step 3**: Consists of adapting the model developed in Step 2 to perform blind predictions, followed by calibration of the GT experiment at Mont Terri, and
- **Step 4**: This optional test consists of implementing the constitutive model developed in Step 1 to simulate the excavation (focusing on the formation of the EDZ), followed by water and gas injection at the Gas Path through Host Rock and Seals experiment (HG-A) tunnel at Mont Terri. Step 4 can be performed in parallel with Step 3.

SFWST researchers from LBNL are participating as DOE's modeling team in this task, continuing their previous work in the related DECOVALEX-2023 gas migration modeling task.

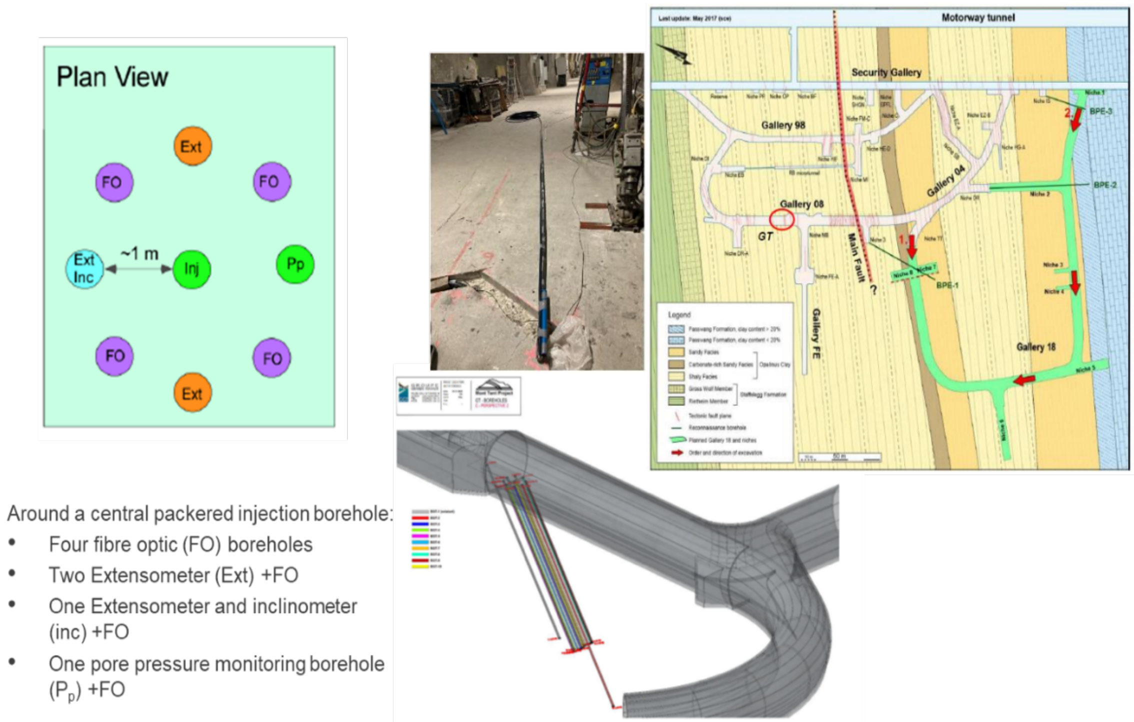


Figure 3.2-17. Location and design of GT Experiment at Mont Terri URL (Nguyen, 2023b).

3.2.3.3 *BATS2 (BRINE AVAILABILITY TEST IN SALT – PHASE 2)*

BATS2 continues the BATS task in the previous DECOVALEX-2023 phase (see Section 3.2.2.5). Kris Kuhlman of SNL again leads this task for the U.S. DOE. The main objectives remain unchanged: To understand the processes and mechanisms governing the migration of gas and brine through the changing EDZ in salt during heating and to improve conceptual and numerical models of these systems and hence the impact on performance and safety assessment. Three main questions will be addressed: (1) Is two-phase flow in EDZ important, or are single-phase or Richards' flow approximations sufficiently accurate? (2) How does permeability evolve due to heating? (3) How do different brine types contribute to brine production? As in the current phase, the focus is on bedded salt at the Waste Isolation Pilot Plant (WIPP) in New Mexico, but the processes generally apply to bedded and domal salt.

Like BATS, the BATS2 task centers on a series of borehole heater tests and gas tracer injection tests conducted in horizontal boreholes in the EDZ surrounding a drift at WIPP. The field data used for BATS2 are associated with several (>4) three-week-long heater tests conducted in 2022-2023 in m-scale arrays of boreholes at increasing temperatures. BATS2 testing is done in the same WIPP tunnel but at a different location. Also, the design of the BATS2 heater array is different from the BATS array, considering lessons learned from the previous experiment. For example, the monitoring boreholes for acoustic emissions and electric resistivity tomography are more spread out, the layout of thermocouples has been improved, the tests have been conducted in a lower stratigraphic interval (MU-0) with more clay content, and the startup before the first test was quicker, which has led to less dry-out in the EDZ. Both heated and unheated arrays of boreholes were monitored. Temperature (thermocouples), brine production, water isotopes, acoustic emissions, electric resistivity, distributed fiber optic strain and temperature, gas tracer concentrations, and brine chemistry have been measured. Figure 3.2-18 shows a schematic drawing of the two heater arrays for the original BATS and for BATS2.

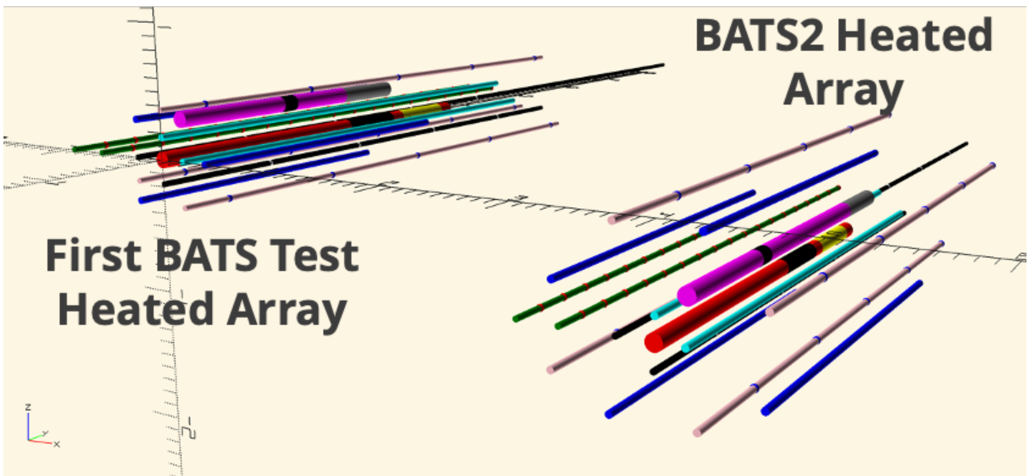


Figure 3.2-18. Schematic of borehole setup for first BATS test versus BATS2 (Kuhlman, 2023).

Like most DECOVALEX tasks, BATS2 is designed with sub-tasks that increase complexity levels.

- **Step 1**: Modeling the thermal response observed during 2022-2023 heating cycles in BATS2 (90°, 120°, 130° & 140°C setpoints already). Thermal responses are easier to predict, but the four target temperatures will better quantify the importance of non-linear thermal effects. Step 1 includes a condensed benchmarking step against McTigue thermoelastic response and two-phase flow. This allows new teams to catch up and may enable existing teams to try new modeling tools or approaches,
- **Step 2**: Includes modeling of salt-specific brine sources, e.g., clay dehydration (water released once the salt reaches a temperature threshold) and fluid inclusion migration (brine associated with migration under thermal gradients),
- **Step 3**: Focuses on modeling gas migration between boreholes during heated and ambient conditions. A packed-off borehole initially held gas pressure, but after repeated heating and cooling cycles, the same borehole allowed gas to flow into the salt. Heating the salt temporarily reverses this permeability increase until heating stops. After heating, gas pressure in the source borehole fell, and the tracer gas was subsequently observed in an adjacent borehole. This will likely require the simulation of a two-phase flow system.
- **Step 4**: Models brine production during BATS2 heating cycles, also considering the different potential sources of brine (Step 2) and the changes in gas permeability observed (Step 3).

SFWST researchers from LBNL, LANL and SNL are participating as DOE's modeling teams in this task, continuing their previous work in the related DECOVALEX-2023 task.

3.2.3.4 SANDWICH EXPERIMENT – TASK A

The focus of this task is the Sandwich Experiment conducted at the Mont Terri URL, described in Section 3.1.5.1. This task is led by the German Gesellschaft für Anlagen- und Reaktorsicherheit (GRS). The main objective is to understand and jointly simulate the HM coupled process interactions between the host rock and the engineered shaft seal elements. Shaft sealing systems are designed to block potential pathways of radionuclides between a nuclear waste repository and the biosphere. Their role is to limit the fluid inflow from the adjacent rock or the surface in the early stage after closure of the repository and to delay the release of possibly contaminated fluids from the repository at a later stage. As mentioned before, the sealing function of the Sandwich design relies on layers sealing layer made of bentonite alternating with equipotential layers that are characterized by a higher hydraulic conductivity. Within the equipotential layers, water is evenly distributed over the cross-section of the sealing layers, which means that more homogeneous hydration and swelling of the seals is obtained. Furthermore, any repository water bypassing the seal via the excavation damaged zone is collected and contained in the equipotential layers.

The GRS task lead plans to provide *in-situ* measurements in the host rock and the shaft elements from the Sandwich Experiment (more than three years of measurements available), both from the shaft sinking and the operation phase (Figure 3.2-19). Also available will be results from accompanying laboratory work on the characterization of the hydro-mechanical-chemical (HMC) behavior of the bentonites and scale transition experiments of the sealing system (MiniSandwich). Participating modeling teams are asked to conduct a combination of blind prediction and model calibration with measurement data, on different scales, followed by prognosis simulations for PS/SA impact evaluation. The model comparison and improvement expected from this task are expected to lead to increased reliability of performance and safety assessment predictions for shaft sealing systems.

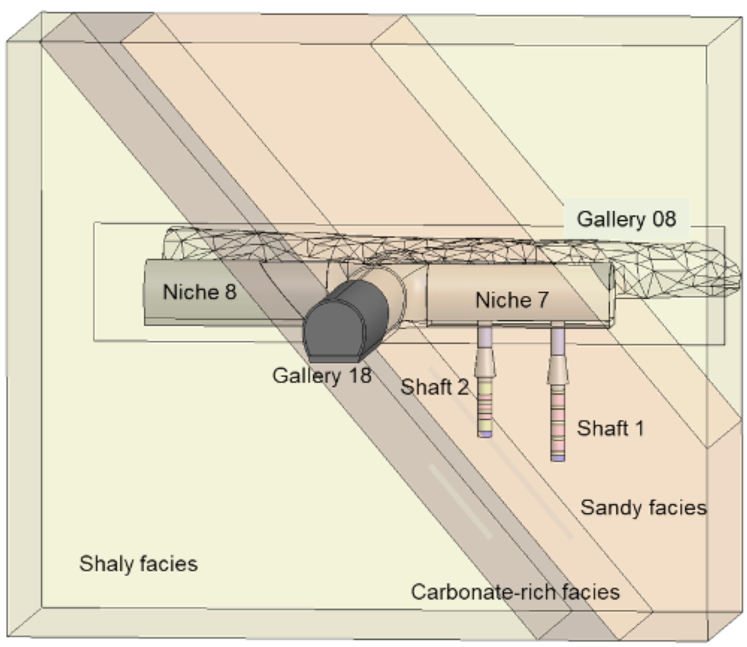


Figure 3.2-19. Schematic of the two shaft geometries in the SANDWICH experiment (Friedenberg et al., 2023).

An incremental approach to the development of this task is proposed based on a stepwise increasing level of complexity:

- **Step 1**: Focuses on the simulation of laboratory experiments. Experimental data for the characterization of the HM-coupled behavior of the bentonite material are made available to the partners, including swelling pressure and hydration tests. The partners should use these data to calibrate their constitutive models. The benchmark tests (BMTs) then include the simulations of the MiniSandwich and semi-technical scale experiments. Therefore, two-dimensional models will be applied, and the HM-coupled processes will be considered. Based on the partners' calibrations, the first simulations will be executed as blind predictions. Then, the results will be compared and verified against the experimental data.
- **Step 2**: Allows an up-scaling of the numerical models to three dimensions. The focus is on the interaction between host rock and sealing elements, including all HM-coupled processes. The simulation process will comprise the excavation of Sandwich Shaft 1, as well as its re-saturation process. It is aimed at reproducing the pore pressure and stress field changes in the Opalinus clay and the sealing element for a fundamental understanding of the interaction. The numerical results can be verified by comparing them against *in-situ* measurement data.
- **Step 3**: Comprises simulation of the *in-situ* experiment in its entirety. The second shaft will be included in the 3D model, and the pore pressure and stress field interactions between the two shafts will be simulated (Figure 3.2-15). Shaft 2 includes a second bentonite material, which will be incorporated later in his step. In-situ measurements are available for the comparison and verification of numerical results. Finally, the 3D model will be applied for prognosis calculations of the SANDWICH experiment.

SFWST researchers from SNL are participating in this task as DOE's modeling teams.

3.2.3.5 BASISS – BENTONITE AND SAND IN SEALING SYSTEMS

Repository closure is an important issue and requires the installation of seals in several places (galleries, shafts, access ramps) to limit water flow. Radionuclides transfer from the storage cells to the biosphere. In geologic disposal, pure bentonite or bentonite/sand mixtures are widely used for sealing and engineered barriers installed close to the waste. However, one of the main issues associated with seals in low-permeability clay host rocks is caused by the production of hydrogen and the resulting gas pressure build-up in the repository. The permeability of the seal to gas plays a significant role in the potential gas pressure build-up, which increases the risk of damage to the host rock. That is why seal concepts in clay host rocks in countries like Switzerland and France have two requirements for long-term safety: (i) to prevent the flow of water (i.e., low equivalent permeability to water (< 10-11 m/s in France)) and (ii) to be as permeable as possible to gas to avoid the risk of fracturing.

BaSISS is led by the French implementor Andra. The task seeks to evaluate seals made of a sand/bentonite mixture with high sand content, which Andra plans to utilize in their repository concept. Both laboratory and field tests have been conducted to test the seal performance and will be made available to task participants. In particular, the full-scale NSC experiment at the Meuse Haute/Marne URL (with a seal made of 40% bentonite MX80 and 60% sand) has been emplaced and saturated since January 2014 (Figure 3.2-20). The seal section of the experiment is 5.1 m long (in between two concrete plugs) and 4.6 m in diameter. More than 300 sensors have been placed into the seal, and over 100 in the near field in the Callovo-Oxfordian claystone. The overall objective of BaSISS, using the provided lab and filed data, is to adapt/develop hydromechanical models necessary for the assessment of the evolution of an installed sand/bentonite mixture seal with high sand content and the resulting sealing ability of the seal (water and gas permeability), during saturation and under gas flow. Understanding and modeling the flow of gas through the seals is paramount to demonstrating the robustness of such seals.

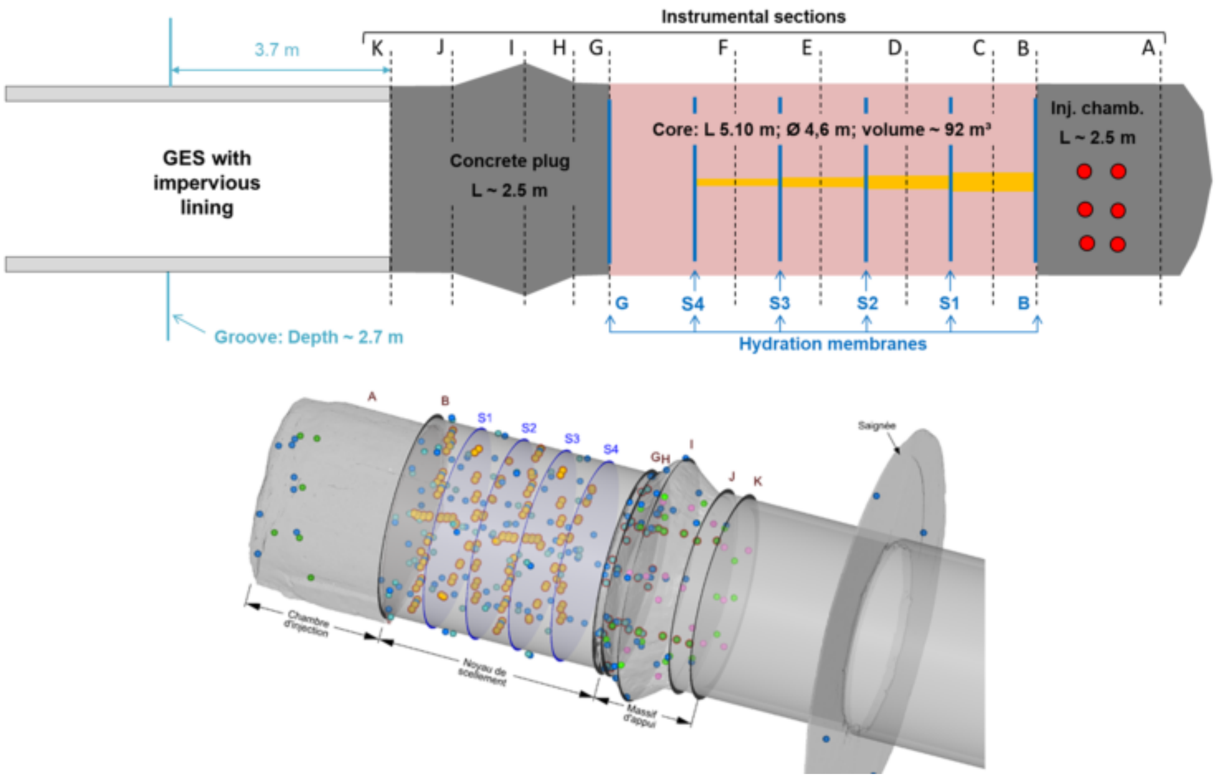


Figure 3.2-20. Top: Schematic showing the seal testing section of the NSC experiment situated between two concrete plugs. Bottom: Sensor locations for pressure and saturation (Plúa and Armand, 2023).

An incremental approach is proposed for developing this task, from sample to *in-situ* scale.

- **Step 1**: Modelling of hydration & gas injection on sand/bentonite mixture sample
  - Laboratory tests performed at BGS,
  - Process analysis and calibration of the model during saturation and gas injection,
- **Step 2**: Modelling of the hydration and water & gas injection test on sand/bentonite mixture in NSC
  - **Step 2a**: Modelling the hydration phase
    - Interpretation (or blind prediction + interpretation),
  - **Step 2b**: Modelling the performance test to water
    - Blind prediction and interpretation,
  - **Step 2c**: Modelling the performance test to gas
    - Interpretation (or blind prediction+ interpretation

There are currently no SFWST researchers participating in this task.

3.2.3.6 FRESCIP – FRACTURED ROCK EXTRAPOLATION, SUITABILITY CRITERIA, AND INFLOW PREDICTION

This task is motivated by a unique data set to be provided by the Finnish implementor POSIVA OY. The Finnish program has already selected a site, submitted a license to operate, and started constructing its Onkalo disposal facility at Olkiluoto. These recent activities provide relevant new data from pilot hole and deposition tunnel investigations, such as fracture frequencies, fracture trace maps, and groundwater inflows. These new data are in addition to previous data obtained from less dense measuring campaigns, such as the site characterization data from earlier site investigation stages. Looking at these new data sets together allows comparison of previous and new fracture data and understanding whether the additional learnings from dense tunnel data impact the PA modeling. Are there surprises, and how do they affect PA predictions? How best to conduct performance confirmation and performance adjustment? Are there lessons learned concerning the need for scientific investigation during the construction stage?

FRESCIP proposes to use the Finnish data sets and repository design to develop and test alternative modeling concepts and methodologies such as DFN and channel network model (CNM), among others. The models will be used in simulations that match *in-situ* hydraulic measurements and fracture mapping in tunnels to aid (a) the decision-making processes by estimating suitable rock volumes for waste storage and optimizing deposition tunnels/holes layout as a function of fracture network characteristics and local stress/pressure/flow conditions, and (b) the evaluation of fluid flow conditions at deposition holes and tunnels to estimate potential radionuclide leakage from waste canisters into the geosphere, as input to regional flow and transport calculations in a repository safety assessment. The task is interested in a staged approach to exercising models at different scales, starting from site descriptive scale before pilot hole drilling to pilot hole investigation, moving from pilot hole investigation to deposition tunnel construction, then moving from deposition tunnel construction to deposition hole placement, and ending with an estimation of post-closure inflow conditions in deposition holes and tunnels according to the Swedish and Finnish repository design. All but the last stage can be compared with measurements. The task is led by the Swedish regulator SSM, Uppsala University in Finland and Clearwater Hardrock Consulting. For example, for the type of data available for this task, Figure 3.2-21 shows fracture traces from a mapping of the Demonstration Area at Olkiluoto.

The proposed task program includes the following steps, corresponding to the planned stages for the construction of deposition tunnels and deposition holes within the KBS-3 concept for final disposal or spent nuclear fuel in crystalline bedrock:

- **Step 1**: Preparatory compilation of site-specific data and generation of synthetic data. This step will be carried out before the main DECOVALEX task. This step will include a definition of specific data packages to be distributed to the modeling groups in each of the following steps, consistent with the types of data available during the corresponding stage of repository construction. At the same time, the participating teams will prepare their own DFN or alternative models (such as CNM) and develop their calibration or conditioning strategies to be used in this task.
- **Step 2**: Prediction of fracture intersections and transmissivities where they intersect the pilot holes for deposition tunnels, based on a DFN or CNM model conditioned to data from nearby tunnels. Predictions are expected to be crude at this stage but representative of the information available at this stage of repository construction.
- **Step 3**: Prediction of full-perimeter intersections of fractures with deposition tunnels and qualitative inflows based on additional data from the pilot holes for deposition tunnels. Data for comparison will come from either the actual site model or the synthetic dataset. It is expected that predictions at this stage will still be of considerable uncertainty.

- **Step 4**: Prediction of fracture intersections and transmissivity in pilot holes for deposition holes. Data for comparison will again come from the actual site model or the synthetic dataset.
- **Step 5**: Predictions of inflows to deposition holes bored in suitable locations based on previous analysis steps and comparison to observations.
- **Step 6**: Predictions of post-closure flow and transport resistance. Comparison (in the case of the synthetic dataset) to modeled results.

SFWST researchers from LANL are participating as DOE's modeling teams in this task.

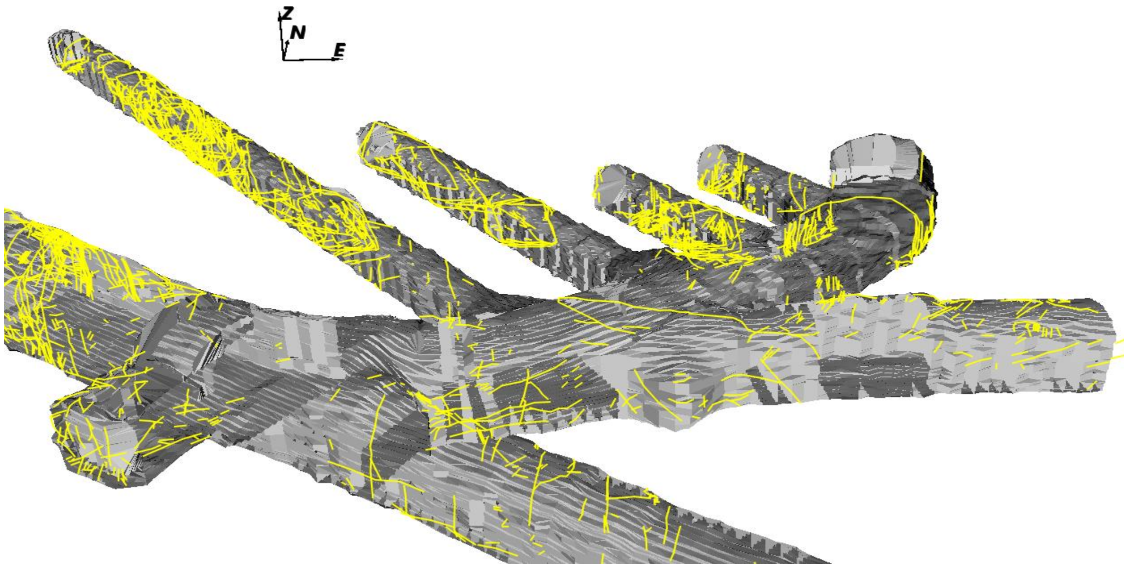


Figure 3.2-21. Fracture traces mapped in the Demonstration Area at Olkiluoto (Geier et al., 2023).

3.2.3.7 ANALOG – MULTISCALE LONG-TERM RADIONUCLIDE TRANSPORT AT CIGAR LAKE URANIUM ORE BODY

Natural analogs provide additional support to the development of safety cases for geologic disposal. The spatial-temporal scales of natural analogs may cover tens to thousands of meters and millions of years and are thus well beyond the scales of experiments conducted in URLs, which typically extend up to tens of meters and tens of years. Through the study of the Cigar Lake natural analog (and possibly another analog site referred to as Kiggavik analog), the ANALOG task seeks to understand the processes and mechanisms of solute transport in clay barriers and fractured rocks at spatial-temporal scales commensurate with the post-closure safety of geological disposal of radioactive waste. This task is led by the Canadian regulator CSNC.

The Cigar Lake deposit is located at approximately 450 m depth at the unconformity between the overburdened sandstone and the basement gneiss. The Cigar Lake uranium mine is unique due to a thick halo of clay minerals that envelopes the ore deposit and provides an analog to the widely used design of engineered clay barriers for nuclear waste disposal (Figure 3.2-22). The clay minerals were reported to be formed by hydrothermal processes dating back to the initial stage of uranium mineralization (approximately 1.3 billion years ago). Uranium is highly enriched in the ore, averaging about 13%, with a maximum of around 66%. I-129 is produced by spontaneous fission of U-238 or neutron-induced fission of U-235. Field measurements can be used to investigate the transport of *in-situ* produced radionuclides in the ore body, which allows developing and calibrating models of radionuclide transport in the clay halo and the near-field rock and far-field rock. The coupled results of field measurements and models enhance our understanding of the mechanism of transport, evaluation of the performance of the clay barriers and host rock, and our ability to conduct performance assessments.

Experimentally measured concentrations of U, I-129, and I-127 in a continuous series of core samples drilled sub-vertically around the Cigar Lake uranium ore body will be available to the participating teams. Test data will be available for vertical profiles of both U and I-129 concentrations in the rock mass. The proposed task comprises the following steps:

- **Step 1**: The transport of conservative tracers is primarily governed by diffusion in the clay barriers. For dense clay barriers, as observed in the Cigar Lake mine, it is necessary to characterize and quantify the diffusion coefficient in the pore space. This step explores different approaches to determining the effective diffusion coefficient for I-129 in the clay barriers.
- **Step 2**: This step investigates the source term for the isotope I-129 in the ore body. Spontaneous fission of U-238 will yield isotope I-129, which has a half-life of 16 Ma. Secular equilibration is generally believed to hold in such systems. However, due to its highly labile nature, iodine will migrate outwards into the surrounding medium (bleaching). As such, the secular equilibration is broken because the system is not isolated but connected to the environment. In this step, mechanistic models are developed to estimate the source term for I-129 using concentrations of U-238 under different bleaching rates. Using this source term, participants develop models to predict the equilibrium concentration profile of I-129 for pre-determined boreholes using experimental results of U and I-129 for calibration of the models.
- **Step 3**: A far-field model is developed for the Cigar Lake mine site. The far-field model is informed by the results obtained from the near-field model, which is calibrated with borehole measurements. Hydrogeological parameters of the geological formations will be provided and then used for the assessment of the key metrics, for example, the mobility of other isotopes of concern such as C-14 or Cl-36 or others, the concentrations of I-129 at the surface or in a hypothetical groundwater well, and critical characteristics of the clay halo that influence 129 transport identified through a sensitivity analysis.
- **Step 4**: The Cigar Lake site has undergone nine glacial cycles in the past million years. These cycles profoundly change the THMC regime of the Cigar Lake formation. In this last step, modeling the influence of these past glacial cycles on U and I-129 migration is proposed, which would involve some degree of coupling between THMC and transport processes.

If the schedule allows, the task may include a second analog study referred to as the Kiggavik site in Canada, which can serve as an analog for uranium leaching by an oxidative fluid under disruptive FEPs. The Kiggavik deposits contain an estimated 51 million kg U at an average grade of ~0.46% uranium. These deposits have often been interpreted similarly to the Athabasca U deposits. However, recent work suggests that the deposits are related to large-scale metasomatic alteration events.

SFWST researchers from LBNL and SNL participate as DOE's modeling teams in this task.

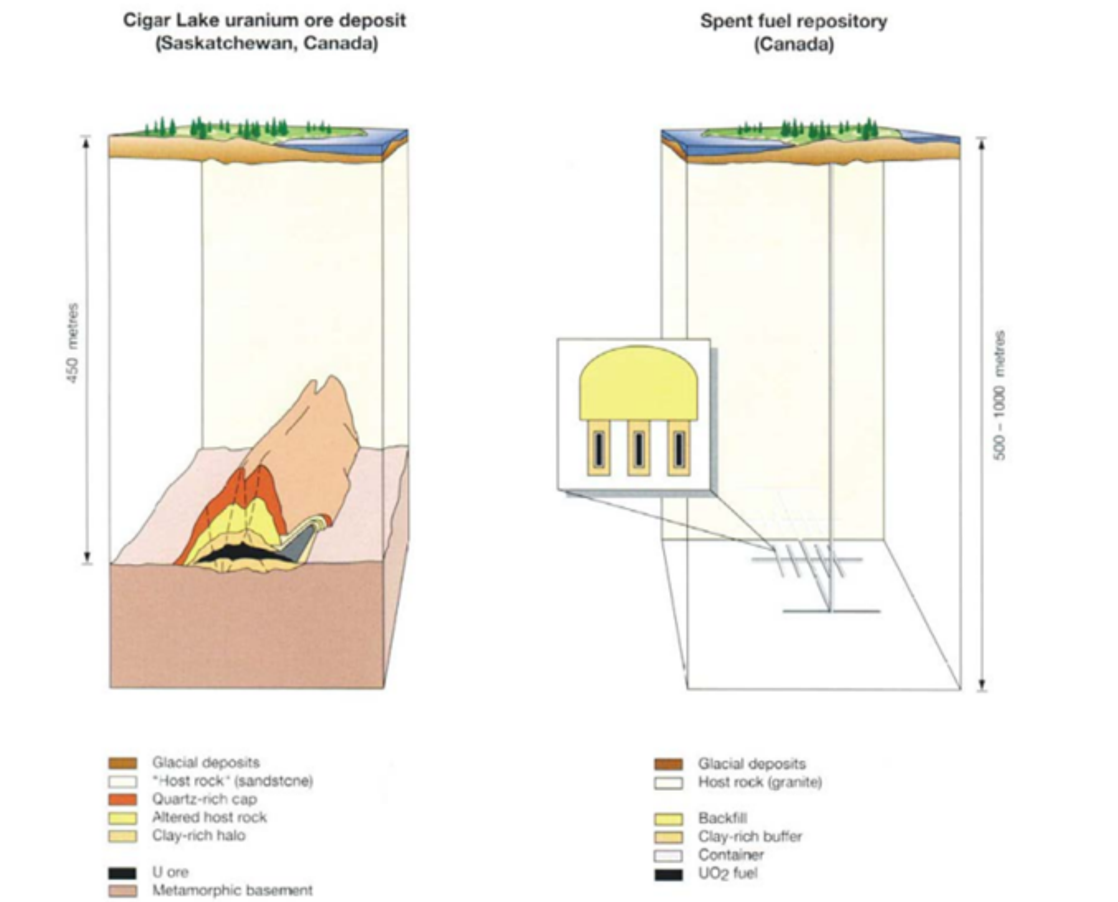


Figure 3.2-22. Schematic of the Cigar Lake Analog versus deep geologic disposal (Nguyen and Li, 2023a).

3.2.3.8 REPOSITORY MODELING AND PERFORMANCE ASSESSMENT 2

This task is a continuation of the PA task in the previous DECOVALEX-2023 phase (see Section 3.2.2.6). Proposed by SNL scientists for the U.S. DOE, the task continues comparing the different approaches to conducting PAs with an eye towards building confidence in the safety cases. By building and using the same generic reference cases, it is possible to make more direct comparisons between the different team approaches and levels of sub-model fidelity. From this collaborative effort, it is expected that a set of highly useful "system modeling" practices will be identified. As was done for DECOVALEX-2023, the new proposal has two subtasks that are run in parallel, one for a crystalline (Figure 3.2-11) and one for a salt reference case (Figure 3.2-23). The major difference is that the current task will be able to push further into UQ/SA. To have the ability to welcome new teams, each subtask is multi-tracked across several steps. Each team is expected to have (or to develop) a working reference case and to participate in UQ/SA activities.

The following steps are envisioned for the continuation of this PA task:

- **Step 1**: Establish repository reference cases. This step allows a new team to develop a reference case as defined in the previously developed task specification (D2023 Task F). New teams are required to run specific benchmarks developed in that task specification for comparison with established outputs. They also have the option to use the DOE models as a starting point,
- **Step 2**: Enhance reference cases. Teams, as they are able, enhance their reference cases with additions identified and agreed upon by the participants. One expected addition for the

crystalline reference case is to include the effects of (or to directly model) stresses due to temperature, earthquakes, and/or glaciation over time on fracture apertures, as informed by process model analysis. Anticipated additions for the salt case are the inclusion of waste package heating, additional comparisons of coupled-process sub-models, and the impact of repository engineering design,

- **Step 3**: Uncertainty quantification and uncertainty analysis (UA). Participants propose and finalize a set of uncertain inputs for the reference case simulations, propagate these uncertainties in realizations, and produce means and confidence intervals of the outputs for comparison. The group may investigate a variety of UQ and UA methods commonly employed in safety assessments, and
- **Step 4**: Sensitivity analysis (SA). Teams conduct SA using an agreed-upon suite of SA methods and metrics, including more traditional methods such as correlation coefficients and linear regression and less common methods such as variance-based methods. Each team may use the PA results from their own model, or perhaps the group may decide to choose one set of PA model results for comparison of SA methods and results.

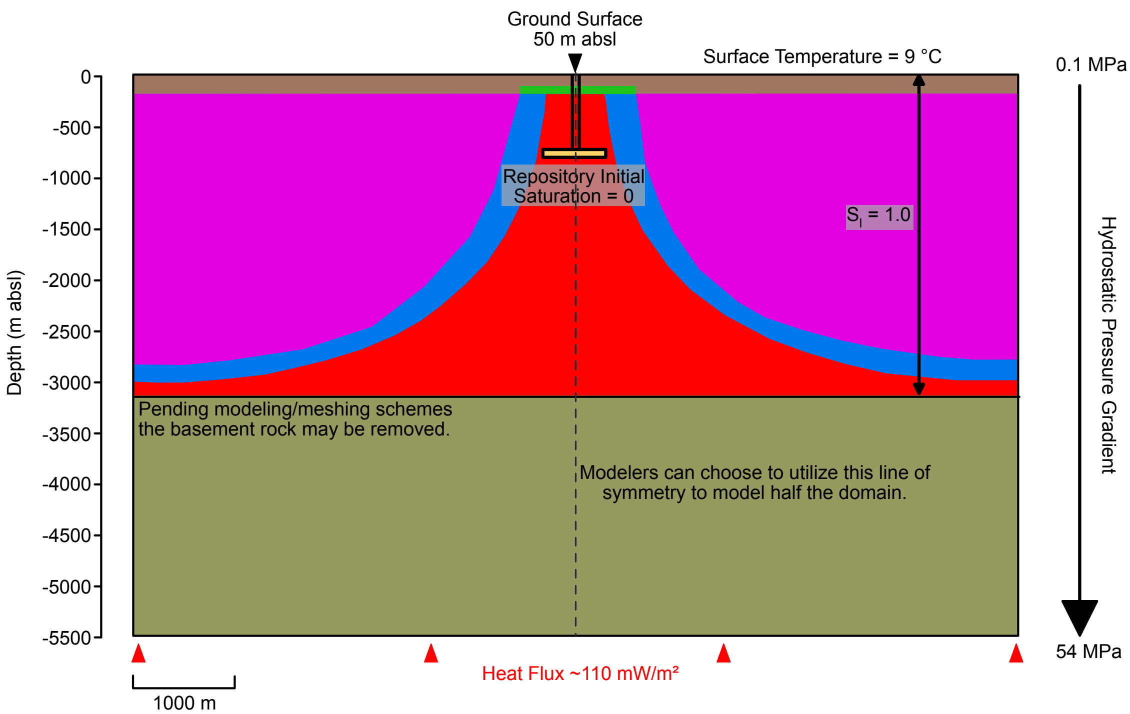


Figure 3.2-23. Generic reference case for a salt repository as developed by the SFWST campaign (Mariner and Jayne, 2023).

3.2.4 DECOVALEX SUMMARY

Benefits of Participation:

- Access to multiple sets of experimental data from different URLs and different host rock environments,
- Opportunities for 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), and
- Opportunity to suggest and/or lead modeling test cases of interest to DOE

Status of Participation:

DOE formally joined the DECOVALEX initiative in 2012, with the start of the DECOVALEX-2015 phase. During this reporting year, DOE scientists finalized several modeling tasks associated with the DECOVALEX phase, referred to as DECOVALEX-2023, which was initiated in early 2020 and ended in December 2023. These tasks included studies on heat and thermal fracturing of low-permeability rocks, bentonite gas migration studies, two full-scale heater tests in argillite and a mudstone, respectively, a brine migration field test in salt, a task focusing on performance assessment methods, and finally, a fundamental task on shear activation in brittle host rocks. A new DFECOVALEX phase started in Spring 2024, called DECOVALEX-2027, with 18 participating institutions and eight research tasks. Two of these tasks are again led by SNL scientists (Kris Kuhlman for Task C, Paul Mariner, Rosie Leone, Tara LaForce, and Richard Jayne for Task E). Also, Jens Birkholzer of LBNL continues to serve as Chair of the DECOVALEX project, which will help ensure that DECOVALEX tasks remain important to DOE's R&D goals.

Outlook:

As discussed in Sections 3.2.2 and 3.2.3, many of the tasks in the most recent DECOVALEX-2023 and in the current DECOVALEX-2027 phase are of high relevance for SFWST, and given the relatively small annual membership fee, the benefit of participating in DECOVALEX remains very high.

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3.3 GRIMSEL TEST SITE PROJECT

The GTS is a URL situated in sparsely fractured crystalline host rock in the Swiss Alps. The URL was established in 1984 as a center for underground R&D supporting a wide range of research projects on the geologic disposal of radioactive waste (Figure 3.3-1). GTS provides an environment analog to a repository site, thus allowing the development and testing of equipment, methodology, and models under fully realistic conditions (www.grimsel.com). GTS is a research facility and not a potential repository site, though investigations may utilize a wide range of radioactive tracers. As the site operator, Nagra has organized most experimental activities in the URL as multinational collaborative projects, which typically include several partners from Europe, Asia, and North America. Participation in these collaborative projects requires a formal agreement between Nagra and its partners. As discussed below, DOE has been quite involved with GTS activities. For example, DOE was a partner in the CFM Project at GTS from 2012 through 2015. DOE also participated in the FEBEX-DP at GTS until its official close in 2018. Since then, SFWST informally continued selected FEBEX-DP activities, for example, using FEBEX-DP data to improve modeling capabilities and using FEBEX-DP samples for further analysis (Section 3.3.1). SFWST is one of several international partner organizations engaged in the high-temperature heater test (HotBENT), which started operating its heaters at the target temperature in May 2022 after years of planning and installation (Section 3.3.2).

GTS also offers other collaboration opportunities that SFWST has not currently tapped into. Examples are the Long-Term *In-situ* Test (LIT) and the *In-situ* Bentonite Erosion Test (i-BET) as part of the CFM Project, the Gas Permeable Seal Test (GAST), the Borehole Sealing Test (SET), and the Materials Corrosion Test (MaCoTe), all of which have been ongoing for a while and are moving into interesting project phases. These ongoing tests and two planned new experiments (Advanced Corrosion Test, ACT; Muon Tomography Proof-of-Principle Project, MUT) of potential interest are further described in Section 3.3.3.

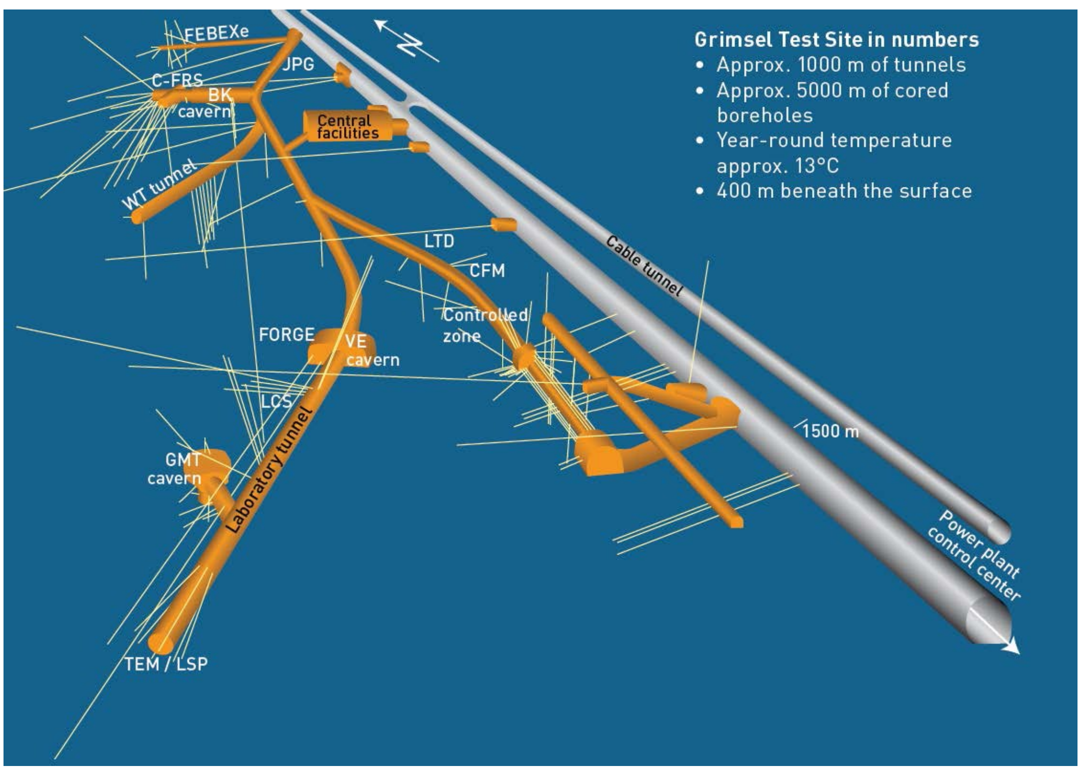

Figure 3.3-1. 3D view of layout of the Grimsel Test Site in Switzerland (Nagra, 2010).

3.3.1 FEBEX DISMANTLING PROJECT

3.3.1.1 OVERVIEW

The FEBEX Full-scale Engineered Barrier Experiment was an international project to study the behavior of a bentonite-based engineered barrier in a crystalline repository. It consisted of an *in-situ* test at the GTS, a mock-up operating at the CIEMAT in Madrid, and a broad portfolio of associated modeling work. The *in-situ* test operated under natural re-saturation conditions for almost two decades (Figures 3.3-2). The overall objective of the *in-situ* test was to evaluate the long-term performance of the EBS and, to a lesser degree, of the near-field crystalline rock, with emphasis on the thermal evolution and the hydrological, mechanical, and chemical evolution as a result of thermal perturbation. The FEBEX *in-situ* test was the longest-running full-scale heater experiment in the world, providing a unique data set for the transient behavior of a heated repository. A fixed temperature of 100°C was maintained at the heater/bentonite contact while the bentonite buffer slowly hydrated with the water naturally coming from the rock. As shown in Figure 3.3-2, the test comprised two individual heater sections placed horizontally into a tunnel at GTS. In total, 632 sensors of diverse types were installed in the bentonite barrier, the rock mass, the heaters, and the service zone to measure the following variables: temperature, RH, total pressure, stress, displacement, and pore pressure.

The *in-situ* test was partially dismantled in 2002 after five years of heating. The first one of the two heaters was removed, and the materials recovered (bentonite, metals, instruments, etc.) were analyzed to investigate the different types of processes undergone. In contrast, the second heater continued to operate (Figure 3.3-3). The samples recovered from this first heater experiment provided valuable information on the long-term condition of heated EBS materials, particularly the geochemical alteration of bentonite, which cannot be measured by embedded sensors (Lanyon and Gaus, 2013).

In FY15, about 13 years after the first partial dismantling, Nagra launched the FEBEX Dismantling Project (FEBEX-DP), which removed the second heater and recovered relevant EBS and host rock materials. This provided a unique opportunity for analyzing samples from an engineered barrier and its components that underwent continuous heating and natural re-saturation for 18 years. DOE joined the FEBEX-DP Project as one of the initial partners, together with Nagra, SKB, POSIVA OY, ENRESA, CIEMAT, KAERI, OBAYASHI, Andra, NWS, and SURAO. The objective of FEBEX-DP project was to provide data and to improve understanding of the long-term THMC performance of the EBS components and their interactions with the host rock. This, in turn, increases confidence in the models required for predicting the long-term evolution of the engineered barriers and how their natural environment affects these. The FEBEX-DP Project thus focused on the collection of the following primary data/objectives (Gaus and Kober, 2014; Nagra, 2014):

- Key physical properties (density, water content) of the bentonite and distribution,
- Corrosion on instruments and coupons under evolving redox conditions and saturation states,
- Mineralogical interactions at interfaces and potential impacts on porosity, and
- Integration of monitoring results and modeling

The dismantling project was initially scheduled to be finished by the end of 2016 but then was extended till the end of 2018 to allow for further sample analysis and interpretative modeling. A comprehensive synthesis of FEBEX-DP data analysis and model interpretation is given in Kober et al. (2021). Though the project officially ended in 2018, the data set has still been used to better understand the performance of barrier components that underwent continuous heating and natural re-saturation for a significant period. Samples collected during the dismantling remained available to study the effect of long-term heating and hydration on the key properties of bentonite. Therefore, some project partners, including SFWST researchers, remained informally involved in collaborative research to further the post-dismantling analysis and modeling interpretation. For example, THM/THMC modeling of the FEBEX *in-situ* test was conducted as Task 9 in the SKB EBS Task Force. LBNL led the task on the 2D THMC modeling, and SNL contributed to developing the 3D TH model. The task ended in 2022, and the final report of Task 9 was finished in 2023. The modeling work by SFWST was completed with a final interpretation of the THMC data (Zheng et al., 2020) and long-term predictions based on the calibrated THMC model (Zheng et al., 2023a).

Ongoing SFWST work related to FEBEX-DP comprises laboratory-scale experiments conducted at LBNL to study coupled microbial-abiotic processes in heated and unheated bentonite samples (Section 6.1.2). The experimental results revealed that clay materials can sustain microbial communities with the potential for microbial growth over time. However, it is intriguing that the materials from the hot zone of the FEBEX test did not exhibit growth potential within the time frames of these experiments. It remains unclear whether this lack of microbiological activities is due to the heating process, the drying process, or a combination of both. Section 5 of Zheng et al. (2024) gives a detailed description of these experimental activities.

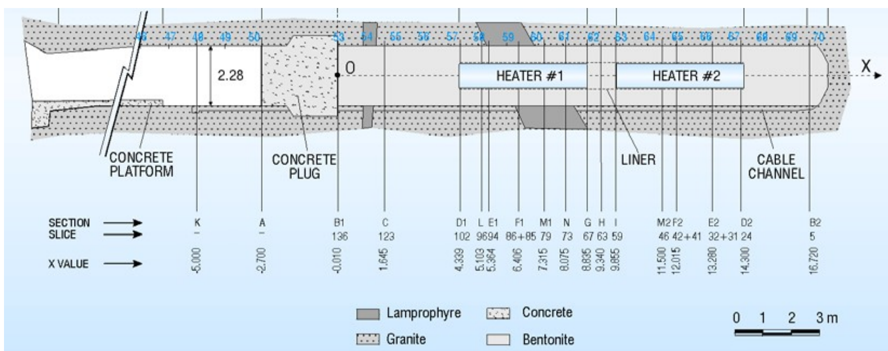

Figure 3.3-2. Schematic cross section of the FEBEX Test at Grimsel Test Site (Nagra, 2014).

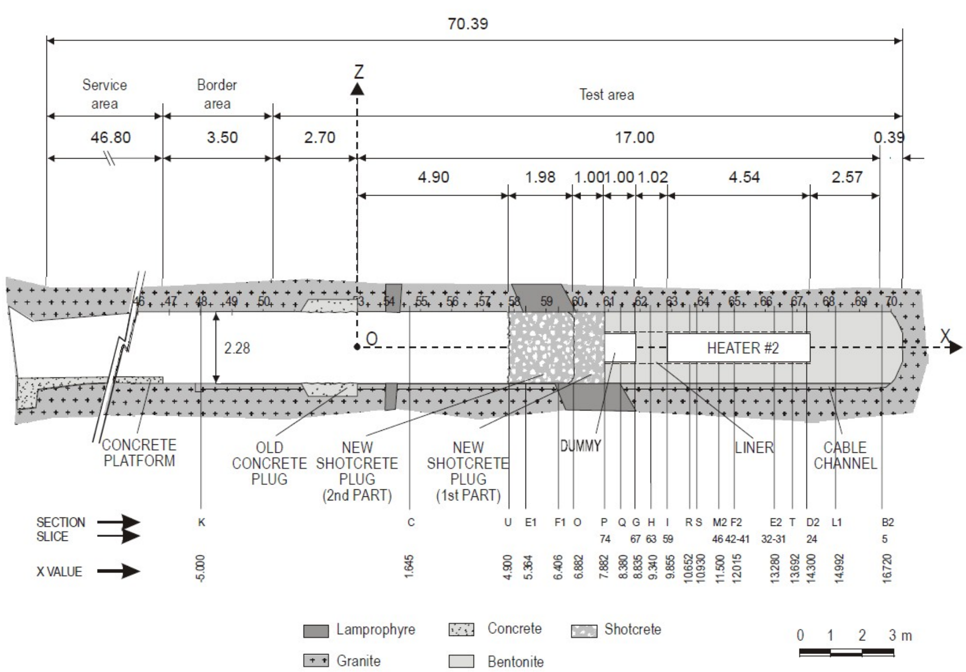

Figure 3.3-3. *In-situ* test configuration following dismantling of Heater 1 (Huertas et al., 2005).

3.3.1.2 FEBEX-DP SUMMARY

Benefits of Participation:

- Access to experimental samples and laboratory investigations from a long-term heater experiment focused on engineered barrier components.
- Opportunity to participate directly in international research groups that analyze samples and conduct modeling work on coupled THMC behavior.
- Opportunity for designing sampling plans as well as conducting own laboratory experiments.

Status of Participation and Outlook:

The FEBEX-DP Project officially ended in late 2018. However, some project partners, including SFWST scientists, are informally continuing their collaboration to further data analysis and modeling interpretation. For example, to support the design of the HotBENT heater test, the THMC model initially developed for the FEBEX *in-situ* test was subsequently modified to consider a much higher heating temperature of 200°C. The THM and THMC modeling activities related to the FEBEX-DP experiment have been embedded in other international initiatives, like the SKB EBS Task Force and the DECOVALEX-2019 Project, but all of these have now ended. The only work related to FEBEX-DP in FY24 comprises the laboratory-scale experiments conducted at LBNL to study coupled microbial-abiotic processes on bentonite samples exposed to 18 years of heating and this work was completed in FY24.

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3.3.2 HOTBENT – A FULL-SCALE HIGH-TEMPERATURE HEATER TEST

3.3.2.1 OVERVIEW

Several international disposal programs have been conducting research activities to understand if clay-based barriers can withstand temperatures higher than the 100°C threshold for bentonite performance usually assumed in advanced repository designs. For example, the SFWST campaign has been investigating the feasibility of direct geological disposal of large dual-purpose DPCs currently in dry storage (Hardin et al., 2014), which would benefit from much higher emplacement temperatures. The performance of bentonite barriers in the <100°C temperature range is underpinned by a broad knowledge base built on laboratory and large-scale *in-situ* experiments. Bentonite parameter characterization above 100°C is sparser (especially for pelletized materials). At temperatures above this threshold, a potentially detrimental temperature-driven physicochemical response of materials (cementation, illitization) may occur, the characteristics of which are highly dependent on, and coupled with, the complex moisture transport processes induced by strong thermal gradients. The impact of such complex processes on the performance of a repository cannot be realistically reproduced and properly (non-conservatively) assessed at a smaller laboratory scale.

Such an assessment needs to be conducted by large *in-situ* URL experiments, where the most relevant features of future emplacement conditions can be adequately reproduced.

Starting in 2015, options for a targeted high-temperature experiment (150°C to 200°C) in a crystalline environment were actively pursued under the leadership of Nagra with several international partners, including DOE (Vomvoris et al., 2015). In FY16, Nagra and partners proposed a new collaboration effort called the HotBENT experiment, a full-scale high-temperature heater test using the well-characterized FEBEX drift at GTS, which has been empty since the FEBEX dismantling in 2015. The benefit of such a large-scale test, accompanied by a systematic laboratory program and modeling effort, is that the temperature effects can be evaluated under realistic conditions of strong thermal, hydraulic, and density gradients, which cannot be reproduced in the laboratory. This leads to improved mechanistic models for predicting temperature-induced processes, including chemical alteration and mechanical changes, which can then be used for PA analysis of high-temperature scenarios. The key question is whether higher repository temperatures would trigger mechanisms compromising the various barrier functions assigned to the engineered components and host rock. If the barrier function is (partially) compromised, PA analysis can evaluate whether the reduced performance of a sub-barrier (or parts thereof) would still give adequate performance. DOE's participation in this collaborative effort is expected to be extremely beneficial; substantial cost savings would be achieved in the design of a repository if the maximum temperature of bentonite backfill can be raised with acceptable performance implications.

From FY16 through FY19, Nagra held several planning meetings to discuss the potential partners' interests in the project and to develop a plan/design for the HotBENT project. Potential partners agreed on a common set of objectives as follows: (1) increase database (monitoring, sampling, lab-analysis) and understanding of buffer behavior at high T conditions (up to 200°C conditions at the canister surface), (2) assessment of buffer performance at realistic scales and gradients compared to small scale laboratory tests, (3) evaluate effects and impacts of microbial activities/corrosion processes/gas evolution, and (4) integrate modeling (e.g. THMC) and lab activities (e.g. mock-up experiments). The partners decided on a modular design with several modules that would differ mainly in the type of bentonite, temperature range, design with/without concrete liner, etc. LBNL actively participated in the project planning and design from the very beginning and used THMC modeling work to help the final design of the experiment. A comprehensive report was completed by LBNL scientists to determine the extent of coupled geochemical alterations expected in HotBENT and whether these would lead to measurable changes in bentonite properties (Zheng et al., 2018). The official HotBENT Project started in 2018 once all agreements with the partner institutions had been in place. In addition to DOE and Nagra, the joint project currently has four other full partner institutions (SURAO, NWS, NUMO, and BGE) and five associated institutions (NWMO, BGR, ENRESA, Obayashi, and KORAD).

3.3.2.2 HOTBENT DESIGN AND STATUS

The following description and figures provide an overview of the design and status of the HotBENT experiment. The test was constructed at the end of the FEBEX gallery (drift) that starts at the northern entrance of the Grimsel Test Site (Figure 3.3-4). The gallery is geologically, hydraulically, and geophysically well characterized (Huertas et al., 2005) and has proven realistic conditions for saturation (Villar et al., 2017a,b). The experimental concept builds on previous experiments and large-scale heater tests in granitic and claystone host rock, such as FEBEX at the Grimsel Test Site, EB, HE-E, and FE at the Mont Terri Underground Research Laboratory. The experiment is designed modularly, whereby a module represents a heater rested on a bentonite block pedestal and encapsulated by a granular bentonite backfill (Figure 3.3-5). Modules differ in design temperature, bentonite type, experimental duration, and whether a liner is used. The two modules deepest in the drift are separated from the others by an insulation plug to enable earlier excavation (i.e., after five years, Phase 1) of part of the experiment with minimal perturbations to the remaining modules (which may run as long as 20 years, Phase 2).

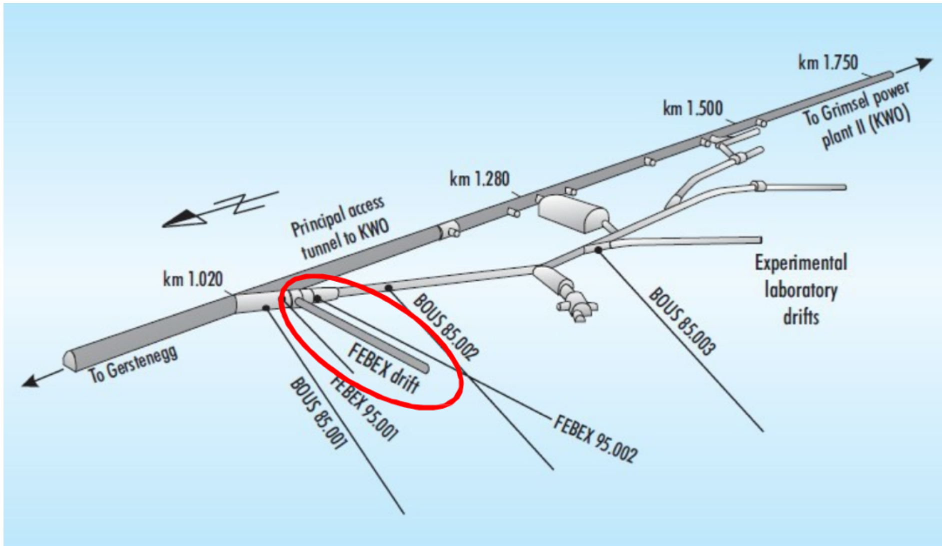

Figure 3.3-4. Location of the FEBEX Drift at GTS (Nagra, 2017).

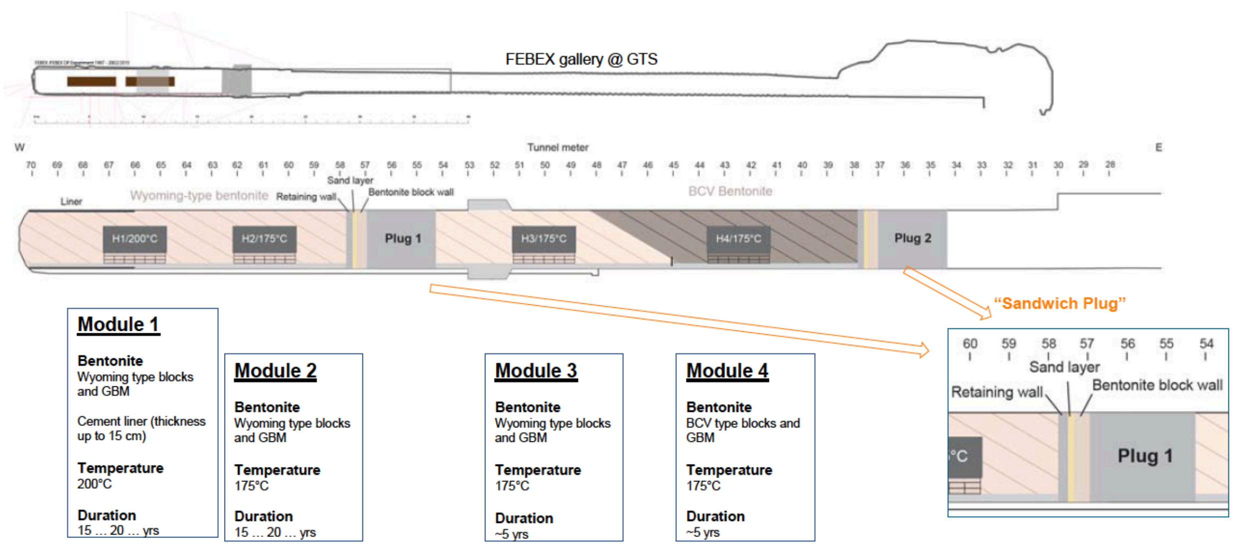

Figure 3.3-5. Final HotBENT design with individual modules (Kober, 2020).

HotBENT features a dense and broad portfolio of monitoring and instrumentation equipment. The THMC evolution of the engineered barrier and the surrounding host rock will be tracked with ~4,100 instruments arranged in 28 monitoring segments along the tunnel axis, measuring properties such as temperature, mechanical pressure, hydraulic pressure, water content, saturation, and humidity, displacements, gas concentration, and gas pressure. HotBENT also includes corrosion studies with metal coupons distributed near the heaters and plans for microbiological characterization. The photo in Figure 3.3-6 shows the complex arrangement of the heater and the sensor equipment before the backfilling of the tunnel with granular bentonite. Note that four boreholes have been drilled in the host rock alongside the heated tunnel which are equipped with multiple packers for segmented forced hydration of the experimental testbed.

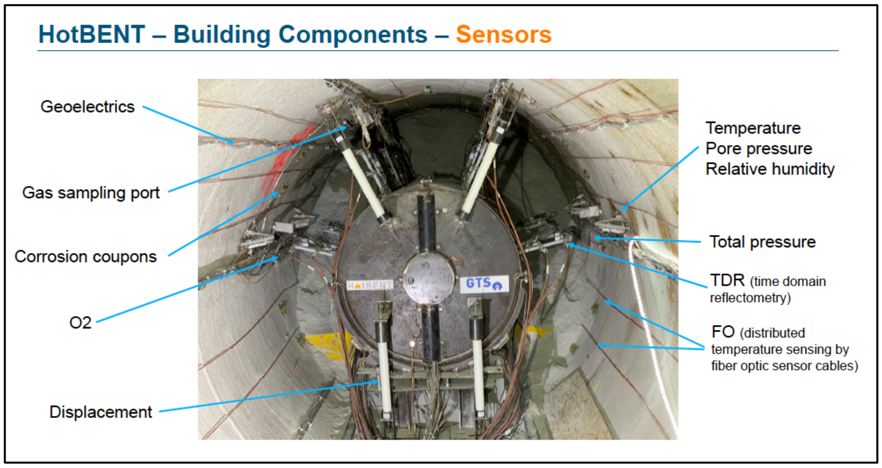

Figure 3.3-6. Photo showing the heater and sensor equipment in the HotBENT tunnel (Kober, 2021).

A detailed timeline for the experiment is given in Figure 3.3-7. After on-site and off-site preparatory work since 2018, the construction of the field test started in February 2020. The construction was completed in August 2021, and on September 9, 2021, all heaters were switched on to an initial power of 300 W per heater. The plan was to increase the temperature stepwise to reach the target temperature in 4.5 months. However, due to the poor accessibility of the test site in winter, the heating was conducted at a slower pace with close monitoring at the site. Eventually, all heaters reached the target temperature in May 2022. Sensors started producing data while the heating was ramping up to the targeted temperature. The variables monitored at the sites include temperature, pore pressure, relative humidity, water content, total pressure, thermal conductivity, heater displacement, plug displacement, and oxygen. Data have been periodically released by Nagra. Because the target temperature was reached later than initially planned, the HotBENT partners decided at the 9th partner meeting in November 2022 to extend Phase I to 2027 (Figure 3.3-7).

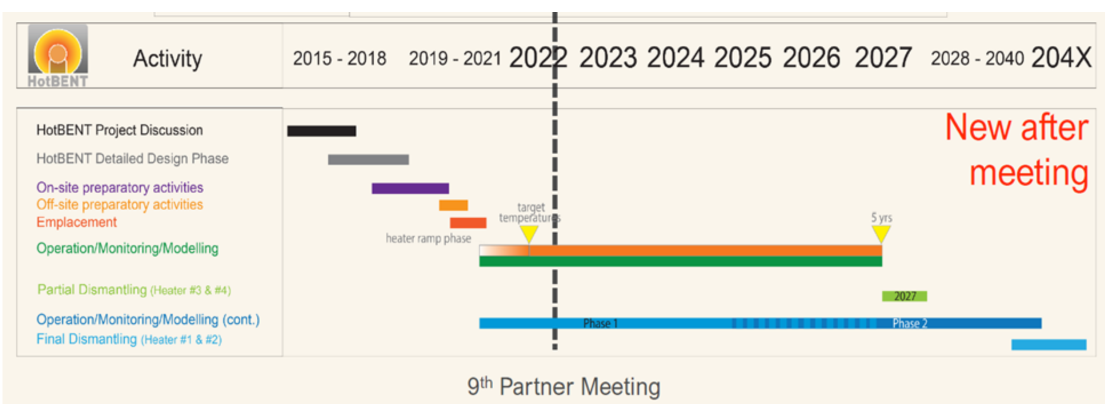

Figure 3.3-7. The planned timeline for HotBENT experiment as planned in 2022 (Kober et al., 2022).

In parallel with the construction of the experiment, Nagra and partners launched a HotBENT Modeling Platform, which includes modeling groups associated with individual partner organizations working on interpretative modeling of the test data. The multi-institutional group is structured to: (a) increase the support provided to the HotBENT experiment and its interpretative evaluation, (b) broaden questions being addressed to advance fundamental understanding, and (c) address modeling issues, specifically the quantification of conceptual uncertainties. In addition, specific expertise and skills of the modeling groups can be used to examine aspects raised by the data collected as part of the HotBENT experiment or to make specific predictions. SFWST scientists from LBNL and SNL are participating in the Modeling Platform. LBNL started with a simple 2D TH model and gradually increased the complexity and dimensionality of the model. In FY24, LBNL finished a 2D cross-sectional THM model to interpret the data collected around Heater #1 and then developed a 3D TH model (see Section 6.1.3 in this report, and for more detailed information see Section 8 in Zheng et al., 2024). In future years, LBNL will develop 3D coupled THMC model, while SNL model will focus on the interaction between bentonite and corrosion products.

3.3.2.3 HOTBENT LAB TESTS

In addition to being the primary THMC modeling group supporting the HotBENT experiment, LBNL conducted a series of bench-scale column tests that mimic closely the heating and hydration conditions of the field-scale experiment (the so-called HotBENT Lab, see Section 6 in Zheng et al., 2024). Two column tests associated with HotBENT Lab#1 (one heated and one unheated) started in June 2019 and were dismantled in December 2020 after running for 564 days. Extensive characterization of heated versus unheated samples has since been conducted. Note that when HotBENT Lab #1 started, the conditions in the field test were not finalized yet. Therefore, HotBENT Lab #1 has some conditions that differ from the field test, for example, the density of bentonite and its hydration pressure were lower than that in the field test. To better support the field test, HotBENT Lab #2 was launched in 2021 with test conditions that are now very close to those deployed in the field test: (1) the bentonite was the same as that used in the field test, (2) the dry density of bentonite after installation was very similar to that in the field test, and (3) the hydration pressure was 2 MPa, which is the expected hydration pressure in the field test after artificially pressurizing the surrounding rocks around the test tunnel with 4 boreholes. HotBENT Lab #2 used similar monitoring methods, including embedded sensors for temperature measurements and electrical resistivity (ERT) and time-lapse CT scans to monitor bentonite evolution. The design of HotBENT Lab #2 is shown in Figure 3.3-8 and more details are given in Section 6 of Zheng et al. (2024). HotBENT Lab #2 test was dismantled after running for 15 months. In FY24, analyses of the clay samples were conducted to measure the water content, dry density of clays and the corrosion of metal coupons. X-ray diffraction (XRD) analysis was also performed but the final interpretation of the data for the mineralogical changes needed more work.

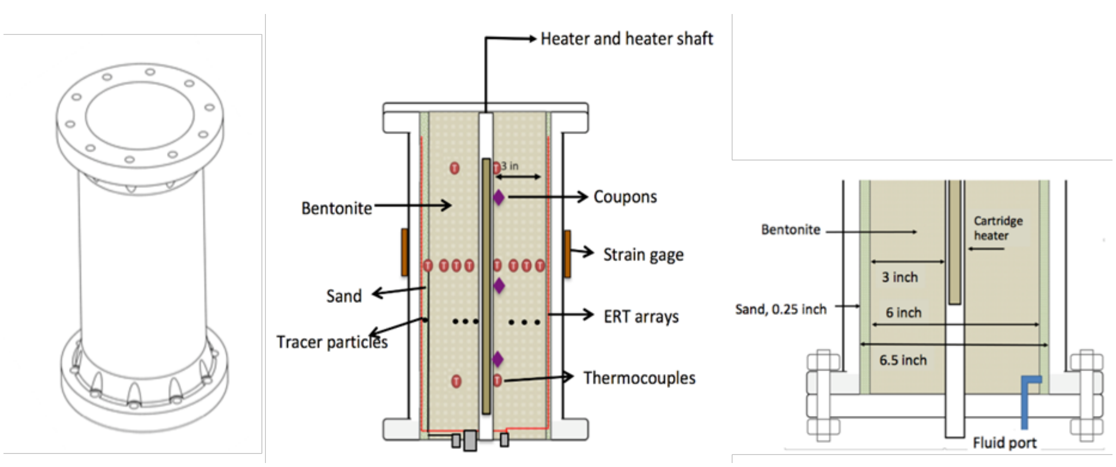

Figure 3.3-8. Schematic diagram of the column design for HotBENT-Lab #2 experiment. Left: 3D rendering of the column exterior; Middle: interior design of the bentonite column showing locations of sensors and the heater; Right: water flow port on the end cap. Tracer particles and coupons are shown at representative locations (Zheng et al., 2022).

Another HotBENT column experiment, HotBENT Lab #3, is currently being planned to further support the field test and modeling work. It differs from HotBENT Lab #2 in the following aspects: (1) The bentonite will be Czech bentonite (BCV) that was used to pack the section around H4 in the HOTBENT field test (see Figure 3.3-5). (2) The hydration pressure will be 0.8 MPa. In the field test, because the hydration indicated by RH data has been quite fast, the hydraulic pressure in the surrounding rocks was only pressurized to 0.8 MPa, which was lower than the initially planned 2 MPa; (3) Instead of using a CT scanner, geophysical monitoring will be done with Electrical Resistivity Tomography (ERT. This is in addition to relative humidity sensors and Time Domain Reflectometry (TDR) to monitor the status of clay. HotBENT Lab #3 is expected to start later in FY24 or early FY25. See Section 6.1.3 in this report for a summary.

3.3.2.4 HOTBENT SUMMARY

Benefits of Participation:

Access to the results of field and laboratory experimental investigations from a long-term full-scale heater experiment focusing on high-temperature (up to 200°C) disposal of radioactive waste. This temperature range is important if DOE is to pursue direct disposal of large dual-purpose waste canisters.

- Opportunity to participate directly in international research groups that analyze monitoring data and conduct modeling work on coupled THM and THC behavior in EBS and natural barrier system (NBS) materials.
- Opportunity for designing the field experiment to DOE-specific needs as well as conducting own laboratory experiments.

Status of Participation and Outlook:

After years of planning, design, construction, and implementation, the HotBENT experiment entered into its heating phase on September 9, 2021. The field test is designed modularly, with individual segments insulated from each other so that part of the experiment may be ended and excavated after 5 years while the remainder of the test keeps running for up to 20 years. Thus, HotBENT will provide valuable data on heat-induced perturbations and alterations in the EBS and NBS of a high-temperature repository for years to come. SFWST scientists have participated in the HotBENT planning from the very beginning and DOE has been one of the founding partners of the HotBENT consortium. SFWST scientists are also participating in the collaborative HotBENT Modeling Platform, and LBNL has been conducting a series of bench-scale laboratory experiments to mimic closely heating and hydration conditions of the field-scale experiment (the so-called HotBENT Lab test).

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3.3.3 OTHER EXPERIMENTS AT GTS

Besides the FEBEX-DP Project and the HotBENT test, other collaboratively conducted experiments at the GTS may also interest DOE/SFWST. Below we briefly introduce some opportunities, including new projects that have recently been proposed (such as ACS and the MUT Project) as well as selected projects that have been running for years but are still available for SFWST to join (such as LIT and i-BET as part of the CFM Project, GAST, SET, and MaCoTe). Because the annual Grimsel Test Site International Steering Committee (ISCO) in 2024 was replaced by a symposium for the GTS 40th anniversary (August 2024), there are no updates for those projects except for ACS and MUT.

3.3.3.1 ADVANCED CORROSION STUDY (ACS)

The ACS is one of the new field experiments proposed recently at GTS. The project is motivated by the concern that sealing (i.e., welding) of the canisters may lead to localized vulnerability. However, the corrosion of sealing materials affected by the transient aerobic period has not been studied in detail. The project, therefore, is focused on investigating the aerobic corrosion of sealing materials under the influence of the bentonite buffer. A series of field and laboratory experiments with various combinations of sealing materials, temperature, and geochemical conditions are planned. The preparatory work has started, and the experiments are expected to start in 2025. NUMO is leading this effort. The second meeting for ACS is scheduled for October 2024.

3.3.3.2 A MUON TOMOGRAPHY PROOF-OF-PRINCIPLE PROJECT (MUT PROJECT)

Muon is an omnipresent particle created in the upper atmosphere, penetrating deeply into the Earth's subsurface. Working like medical x-rays, the application of muon tomography could provide a non-invasive way to detect key geological features (caverns, faults, and fractures) surrounding the nuclear waste emplacement tunnels. A proof-of-principle project has been proposed at GTS to study (1) if muon tomography is a feasible technique for safeguards and safety considerations in a repository, (2) what can be monitored by muon tomography (e.g., spent fuel emplacement chambers, voids, tunnel systems, etc.), and (3) the role of muon tomography in unattended monitoring of a repository infrastructure during its construction and the operational phase. The experimental work will focus on testing the operation of different instruments and detecting known voids and fractures. The project was kicked off in April 2024 and is scheduled to be finished in 5 years. Six work packages have been planned. Work Package 1 comprises a series of modeling efforts to estimate the time needed to detect the large geological features at GTS and evaluate different forms of detectors (planar vs borehole). The design of the field test will be finalized by the end of 2024.

3.3.3.3 EXPERIMENTS ASSOCIATED WITH THE CFM PROJECT

The Colloid Formation and Migration (CFM) Project is a long-term international research project for investigating colloid formation due to bentonite erosion, colloid migration, and colloid-associated radionuclide transport. The CFM project was initiated in 2004 and has operated in four major phases. Using this novel setup, the CFM team conducted 30 colloid tracer tests between 2006 and 2013 in the controlled flow field in and near the shear zone. These experiments evaluated the transport of bentonite colloids with radionuclides from the source to the extraction point at the tunnel wall. More recent CFM Phases 3 and 4 focused on bentonite erosion, colloid generation, and radionuclide transport. Phase 4 (2019-2023) is nearly finished, and Phase 5 is under discussion. Current options discussed for Phase 5 include a possible new migration experiment for RN and colloids in the shear zone and a possible new bentonite erosion test (i-BET2), supported by laboratory and modeling tasks.

DOE joined the CFM Project in August 2012 but ended its official membership in 2015. After that, SFWST researchers collaborated informally with CFM researchers by supplementing the field interpretation with targeted laboratory experiments and modeling studies. There are no SFWST activities directly related to the CFM project. Still, LANL researchers are currently performing a series of experiments to study bentonite clay erosion, coagulation/flocculation, and simulated fracture clogging behavior under controlled conditions. This work is loosely connected with international collaboration efforts conducted in the CFM (i-BET experiment) and FEBEX projects. See Section 6.2.3 in this report for a summary, and for more detailed information, see Section 1 of (Viswanathan et al., 2024).

LONG-TERM IN-SITU TEXT (LIT)

The CFM project started the LIT experiment in 2014 (in Phase 4 of CFM) with the emplacement of a radionuclide-doped bentonite plug into an injection interval CFM 06.002 intersecting the flowing shear zone at the GTS. Three smaller diameter boreholes, CFM 11.001, 11.002, and 11.003, were drilled through the shear zone in roughly a triangular pattern around CFM 06.002 to serve as near-field monitoring boreholes during the LIT. Starting in 2014, the radionuclide-doped bentonite plug was placed in the flowing shear zone for about five years (CFM Phase 3), until 2019 when the ensemble of four boreholes was overcored. Samples obtained from the overcoring were used in a comprehensive post-mortem evaluation of the LIT to determine the disposition of both bentonite and radionuclides in the shear zone at the end of the experiment.

IN-SITU BENTONITE EROSION TEXT (I-BET)

The current CFM Phase 4 centers on the i-BET experiment. The project aims to study bentonite swelling, colloid generation, and radionuclide migration in fractured crystalline rock. It addresses a scenario where a waste package breach allows radionuclides to sorb onto bentonite backfill, which may erode into flowing fractures and carry radionuclides away on colloids. The experimental setup involves bentonite rings emplaced into a borehole around a steel mandrel and sealed at both ends with packers. During the installation of i-BET in late 2018, all bentonite rings were equipped with multiple sensors to monitor the swelling pressure and the water content. Additional boreholes were drilled to monitor the groundwater composition around the source and detect potential bentonite erosion. Near-field sampling was conducted from boreholes about 14 cm from bentonite and far-field monitoring from an extraction borehole 2 m away. For over 1,600 days of monitoring, hydraulic pressure is low and stable. Colloid concentrations significantly increased over the background (Figure 3.3-9). i-BET provides a great opportunity for SFWST to understand and improve the modeling capability for bentonite erosion.

SFWST PARTICIPATION IN CFM

The CFM experiments are unique in that they evaluate colloid-facilitated radionuclide transport in a field setting that mimics a high-level nuclear waste repository scenario. Realizing the benefit of becoming a formal partner, DOE in early 2012 formally applied for a partnership in the CFM Project and was accepted as a new partner in August 2012. The partnership gave DOE and affiliated National Laboratories exclusive access to all experimental data generated by CFM. More importantly, it allowed SFWST researchers to work collaboratively with international scientists in ongoing experimental and modeling studies, and it involved them in the planning of new experimental studies. Like the Mont Terri Project, this type of international collaboration goes beyond the modeling focus of DECOVALEX.

In contrast to both the DECOVALEX project and the Mont Terri project, which comprise a range of experiments covering a wide spectrum of relevant R&D issues, the CFM has a relatively narrow focus, i.e., colloid-facilitated radionuclide migration. In part because of this narrow focus and the comparably high membership fee relative to other international initiatives, DOE decided in 2015 to cancel its participation in the CFM Project. In FY16, a comprehensive synthesis of the current state of knowledge of colloid-facilitated radionuclide transport from a nuclear waste repository risk-assessment perspective was assembled in an overview report by Reimus et al. (2016). The report draws heavily on findings from the extensive and carefully controlled colloid-facilitated solute transport experiments conducted at GTS. The current CFM project partners are from Germany (BMWi/KIT, BGE), Japan (NUMO), Great Britain (NWS), the Republic of Korea (KAERI), and Switzerland (Nagra). SFWST researchers have been closely following the progress of CFM to evaluate whether the ongoing LIT or i-BET experiments would offer important new scientific direction, in which case renewing the previous partnership makes sense. The upcoming CFM Phase 5 may offer additional collaboration opportunities. These will be evaluated when more details on Phase 5 become available.

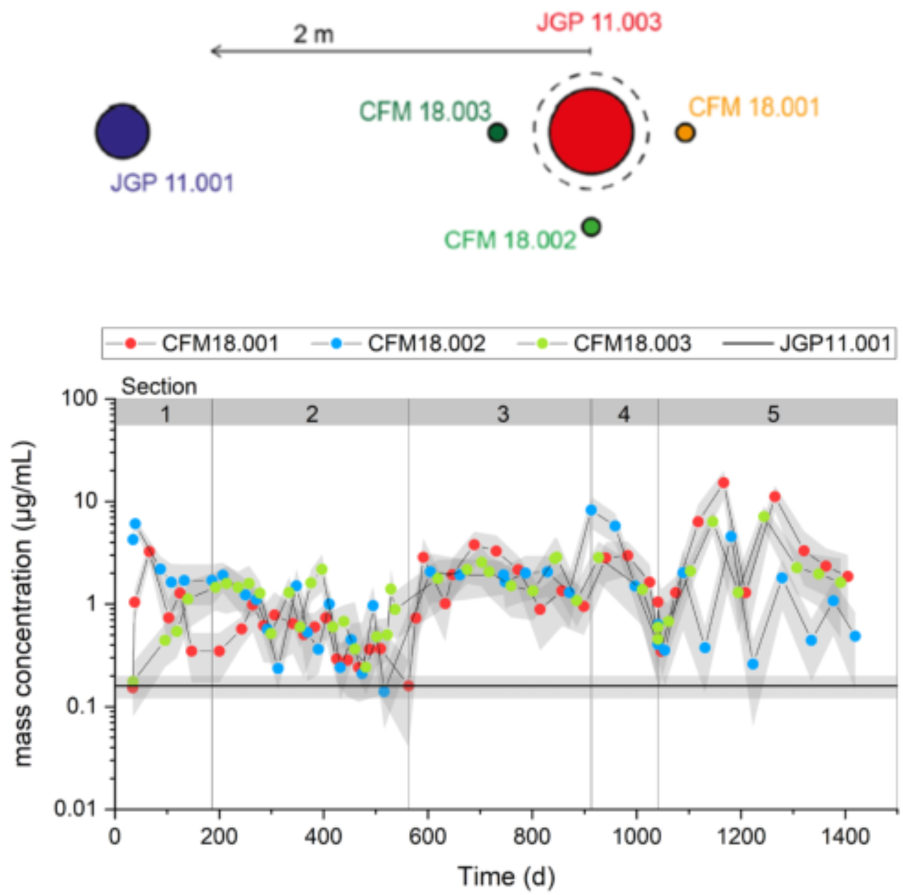

Figure 3.3-9. Monitoring water sampling and colloid concentration at monitoring boreholes (Blechschmidt et al., 2023).

3.3.3.4 GAS PERMEABLE SEAL TEST (GAST)

GAST investigates the performance of bentonite-sand mixtures for increased gas transport capacity (to mitigate pressure buildup from long-term gas generation because of canister corrosion) within the backfilled underground structures without compromising the radionuclide retention capacity of the engineered barrier system (Figure 3.3-10). The objectives of the test are as follows:

- Demonstrate the effective functioning of gas-permeable seals,
- Validate and improve current conceptual flow models for sand/bentonite, and
- Determine up-scaled water and gas permeabilities of sand/bentonite.

Designed and constructed in 2011, the full-scale *in-situ* experiment has been in a slow saturation phase for almost 10 years and is finally reaching full saturation and good homogenization. After a lengthy preparation phase, the long-duration Gas Flow Test (GFT) was finally kicked off on May 2, 2022. The GTF test was planned to last until the second quarter of 2023. Before the start of GFT, the pressure gradient across the sand/bentonite was maintained by a small water injection rate of 0.1 ml/min, with a pressure of 1.8 MPa at one end and a pressure of 1.4 MPa at the other end. The GFT underwent eight phases (see Figures 3.3-11 and 3.3-12). In Phase 2-5, a stable gas flow path was established for a gas mixture with 98% N2 and 2% He (Figure 3.3-11). In Phases 6 and 7, the system was flushed with pure N2 to prepare for a gas tracer test #2 in Phase 8 (Figure 3.3-12).

Nagra started the GAST Modeling Group with simulations using TOUGH2 to match the history of GAST and forecast future test plans. A model using CODE_BRIGHT was also applied to simulate the flow path development due to mechanical effects. GAST is an excellent opportunity to understand gas flow in bentonite-sand mixtures. However, the design of GAST and its objectives are quite similar to the NSC Test conducted at the Bure URL in France, which is at the center of the BaSiSS Task (Bentonite and Sand in Sealing Systems) in the current DECOVALEX-2027 initiative (Section 3.2.3.5). Currently, SFWST scientists are neither participating in GAST or in the BaSSIS Task. If the campaign decides that collaborative field studies of gas-permeable sealing materials are relevant to its mission, both GAST and BaSSIS offer suitable options.

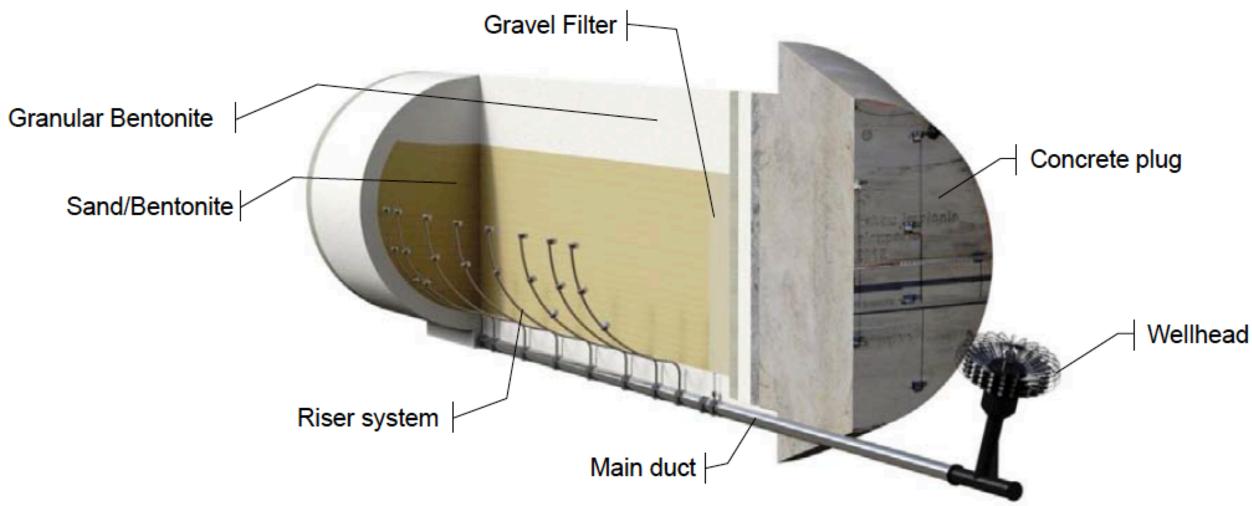

Figure 3.3-10. Schematic illustration of Gas Permeable Seal Experiment at GTS (Reinicke et al., 2020).

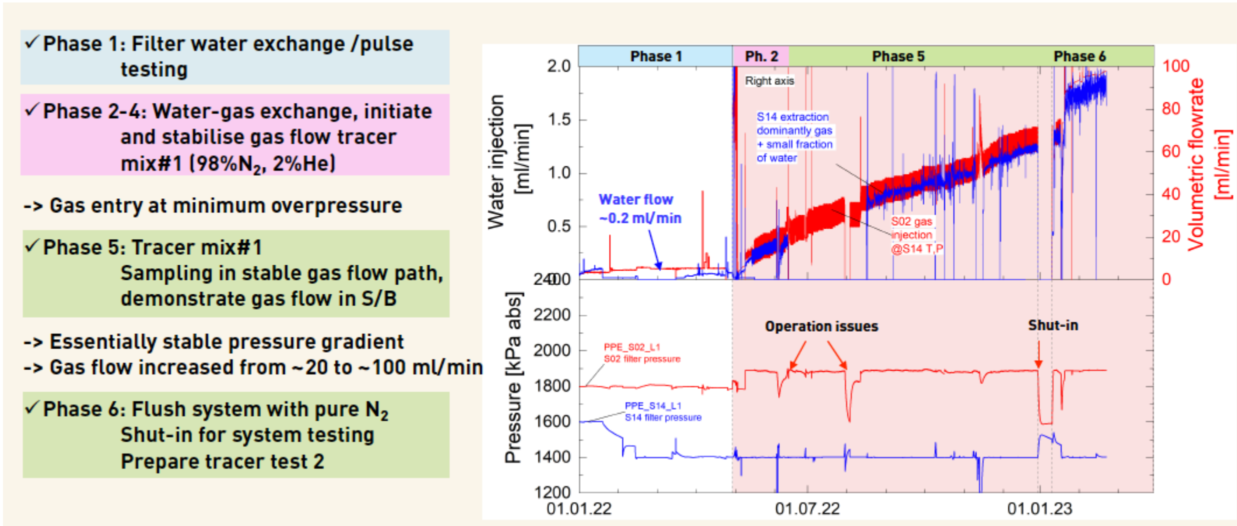

Figure 3.3-11. Phases 1 to 6 in the GAST, and measured water injection rate, gas flow rate, and pressure (Spillmann et al., 2023).

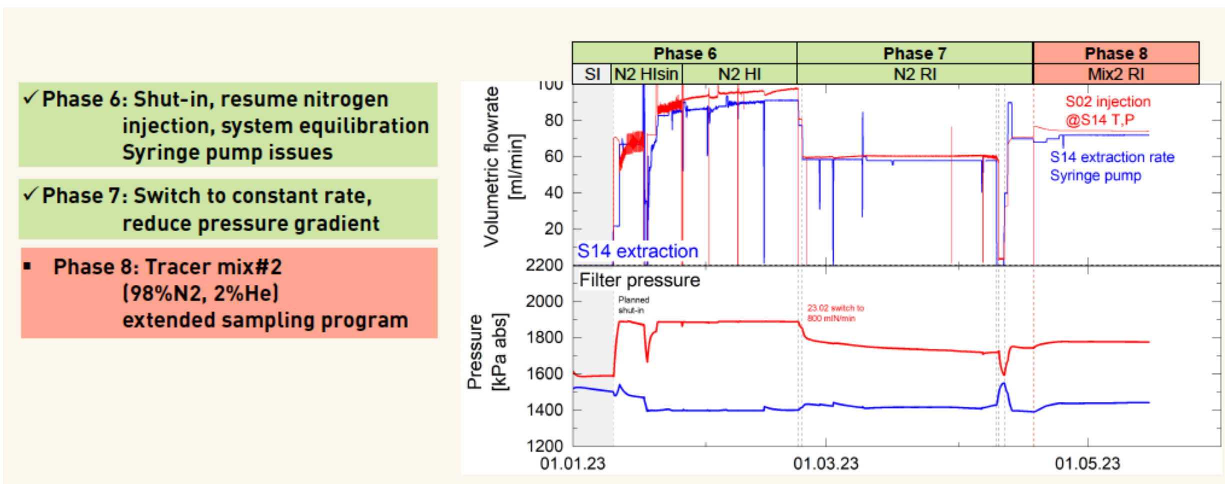

Figure 3.3-12. Phases 6 to 8 in the GAST, and measured water injection rate, gas flow rate, and pressure (Spillmann et al., 2023).

3.3.3.5 *BOREHOLE SEALING TEST (SET)*

NUMO leads the SET to study the performance of a Kunigel-V1-based borehole seal at a realistic scale. The test focuses on the saturation development, the swelling pressure, and the hydraulic conductivity of the borehole seal in a vertical setting within crystalline bedrock. Two vertical boreholes – accessible from both ends – were used for testing a 1-m Kunigel V1 plug. Instrumented packer equipment and high-precision pumps allow for artificial saturation and execution of different hydraulic characterization procedures (Figure 3.3-13). On June 3, 2022, the SET field test was emplaced. Borehole SET 1 was sealed at 7.87-9.13 m and SET 2 at 2.21-3.47 m. Each 1-m long interval was filled with bentonite pellets, resulting in a dry density of 1.21 g/cm³ for SET 1 and 1.15 g/cm³ for SET 2. Injection of Grimsel water was started from pressure tanks with 5 bar pressure. The test has been running for about one year. In SET 1, a slow increase in pore pressure was observed, and the difference between the pore pressure near the upper and lower packer was about 2.5 to 5 bars. Swelling pressure reached about 2 bars in May 2023 and is still developing. In SET 2, the pore pressure gradient across the seal is 3.3-4.4 bars, and swelling pressure only reached 1 bar by May 2023.

NUMO has invited international teams to partner in the experiment and support the project through predictive and interpretative HM modeling. Although hydration tests of bentonite buffer had been conducted before, the SET test differs from other tests in terms of the structure of bentonite: The emplaced mixture consists of 51.3% large almond-shaped pellets, 6.0% small almond-shaped pellets, 17.1% large sheets, and 25.6% small sheets. SFWST should consider joining the modeling team to understand the hydration of bentonite seal because the mixture may have very different hydration behavior than homogeneous bentonite.

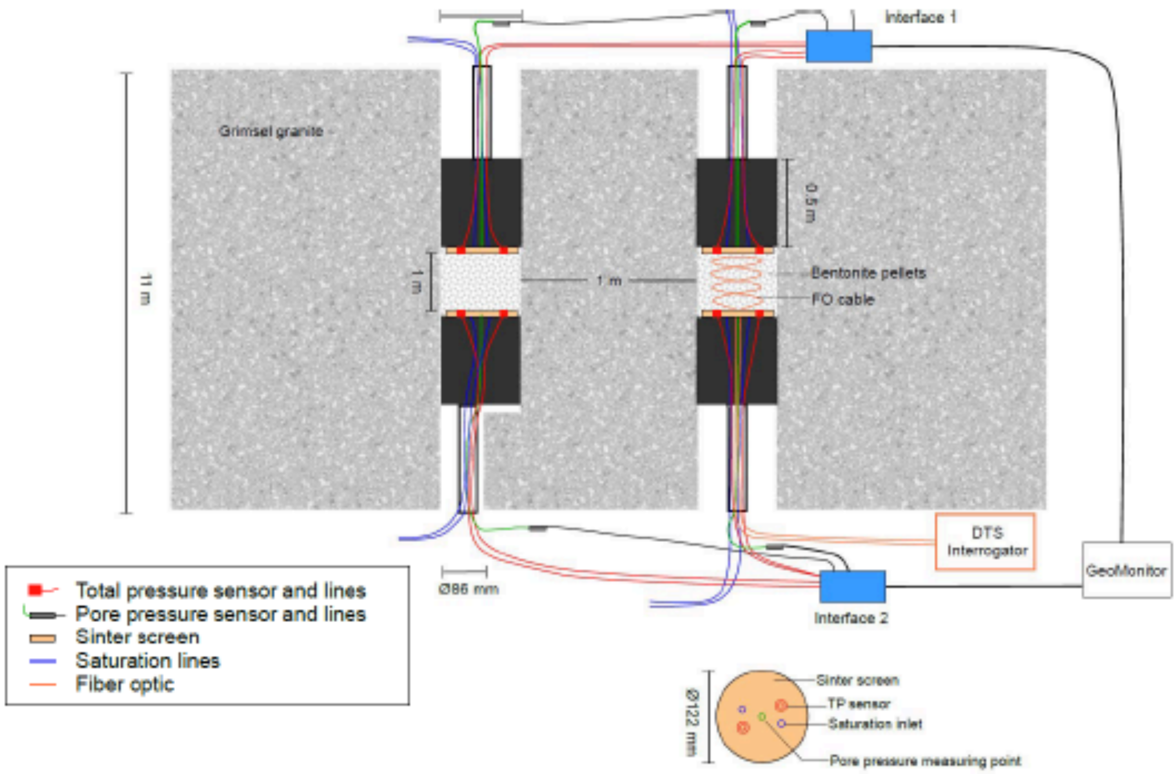

Figure 3.3-13. Schematic illustration of SET Experiment at GTS (Schneeberger, 2022).

3.3.3.6 *MATERIALS CORROSION TEST (MACOTE)*

MaCoTe consists of non-heated and heated experiments to study the *in-situ* corrosion of candidate canister materials embedded in bentonite. Broad aims are as follows (Martin, 2022):

- Obtain *in-situ* corrosion rates under anoxic conditions,
- Study corrosion products and material interactions (metal – bentonite),
- Study the influence of MA, and
- Investigate the influence of heat.

The ongoing *in-situ* experiment comprises a series of specially designed modules (0.3 m long) inserted into a 10 m long vertical borehole and sealed with a double packer system. Each module contains 12 specimens embedded in bentonite with dry densities of either 1.25 or 1.5 Mg/m3

(Figure 3.3-14). Different bentonite types and densities are used, mostly MX-80 bentonite from Wyoming and the Czech BaM lime-magnesium bentonite. Starting in 2014, metal samples have been periodically removed for destructive and non-destructive testing (after 1, 4.5, 7, 10 and 15 years). Currently, the analysis and reporting of 7-year modules are ongoing for the non-heated test, and the removal of 9-year modules is planned for November 2023. The heated test, data analysis, and reporting of results from the 7-year modules are ongoing.

At this point, the experiment offers DOE/SFWST researchers a rich and growing dataset for evaluating corrosion processes in an anaerobic bentonite environment, at ambient and under heated conditions. The current experimental partners (seven) are open to additional organizations joining. The experiment may offer the option of adding material specimens of particular interest to new partners.

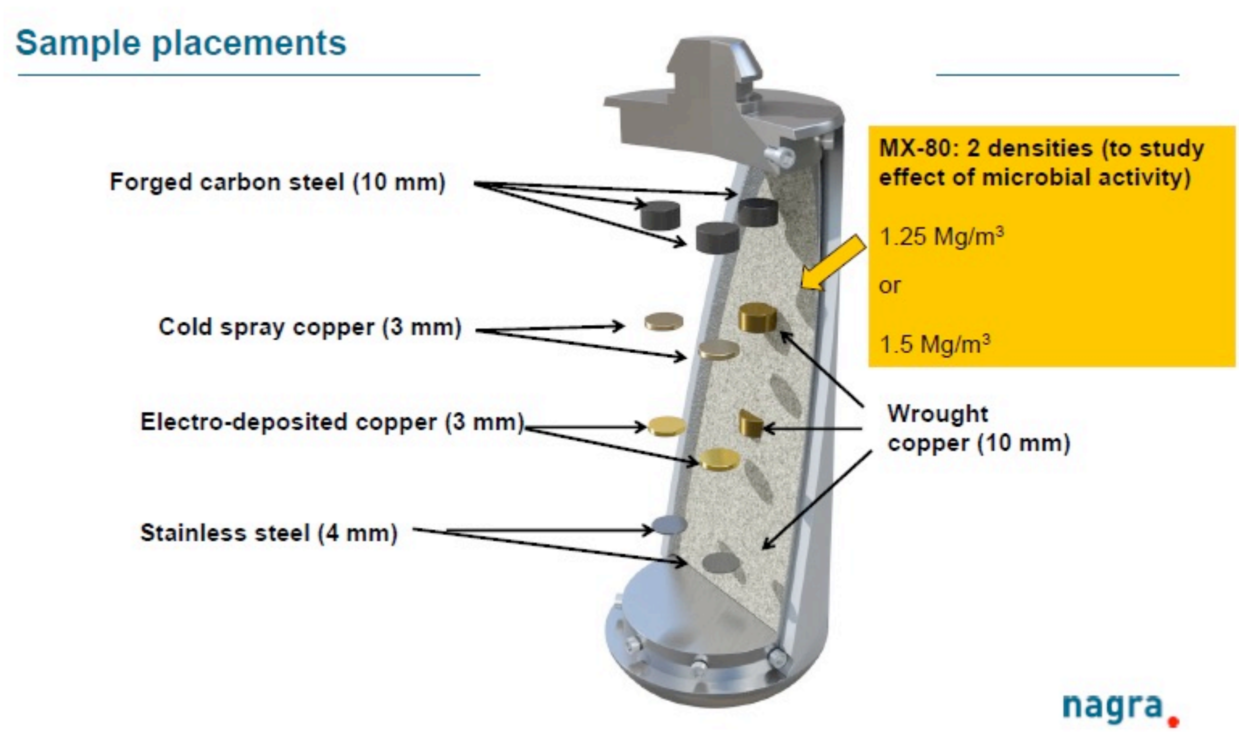

Figure 3.3-14. Schematic illustration of MaCoTe Experiment at GTS (Martin, 2022).

3.4 INTERNATIONAL COLLABORATION INITIATIVES ORGANIZED BY SKB

3.4.1 SKB TASK FORCES

SKB, the Swedish Nuclear Fuel and Waste Management Company, has been organizing so-called Task Forces as a forum for international organizations to interact in conceptual and numerical modeling of performance-relevant processes in natural and engineered systems. There are two task forces: the GWFTS Task Force, initiated in 1992, and the EBS Task Force, initiated in 2004. The EBS Task Force has two parts, one for THM processes and the other for THC processes. Different modeling tasks are being addressed collaboratively, often involving experiments at SKB's Äspö HRL situated in the crystalline rock near Oskarshamn in Sweden. The Äspö HRL consists of a main tunnel that descends in two spiral turns to a depth of 460 m, where various tests have been performed in several side galleries and niches (Figure 3.4-1). SKB collaborates closely with the Finnish repository program; thus, sometimes, SKB Task Force modeling tasks use experiments conducted at the Onkalo URL in Finland (Section 4.8). In recent years, the task forces have moved to include relevant modeling tasks unrelated to the Äspö and Onkalo URLs.

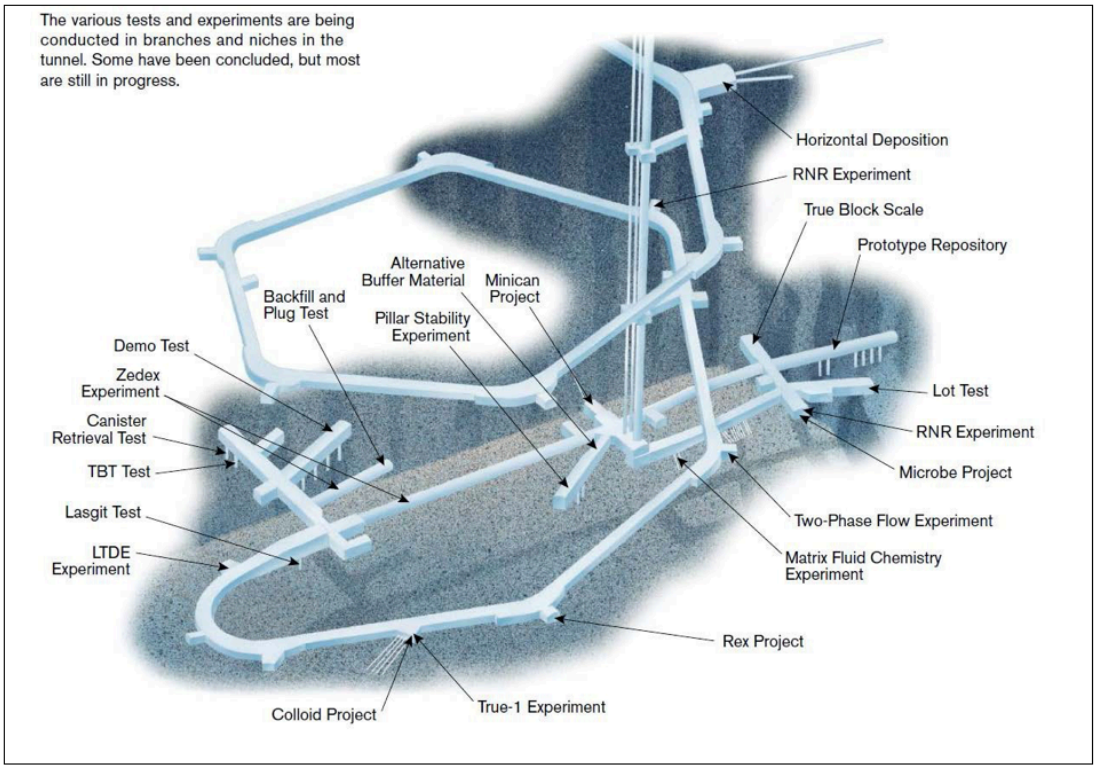

Figure 3.4-1. The layout of Äspö HRL and location of main experiments (Birkholzer, 2012).

Like the other collaborative initiatives introduced earlier in this report, participation in SKB in the Task Forces requires a formal membership agreement. Each participating organization is represented by a delegate; the modeling work is performed by modeling groups associated with these organizations (not unlike the DECOVALEX framework). The task forces meet regularly about once to twice a year. In tasks involving experimental work, task force members interact closely with the principal investigators responsible for conducting experiments. Much emphasis is put on building confidence in the approaches and methods in use for modeling of groundwater flow and migration, as well as coupled THM and THC process, to demonstrate their use for performance and safety assessments.

DOE joined both the GWFTS and EBS Task Forces task forces in January 2014. Other participating organizations in the GWFTS and/or EBS Task Forces are SKB, POSIVA OY, KAERI, CRIEPI, JAEA, Nagra, BMWi/KIT, NWS, NWMO, and SURAO. Regarding the GWFTS task force, SFWST researchers initially conducted simulation work supporting interpreting the Bentonite Rock Interaction Experiment (BRIE) at Äspö HRL, Sweden experiment (FY14 and FY15). In FY17, SFWST's focus shifted to another GWFTS modeling task, which involved diffusion and sorption experiments conducted at the Äspö HRL, Sweden, and the Onkalo URL, Finland. This effort ended in FY20 and instead, SFWST researchers have started participating in a new GWFTS Task 10, which addresses modeling challenges related to multi-scale flow channelization in fractured crystalline rock and validation of fracture network models (Section 3.4.2). Regarding the EBS Task Force (Section 3.4.3), SFWST researchers initially focused on simulation studies related to a full-scale demonstration experiment at Äspö HRL, the Prototype Repository. Starting in FY20, SFWSTs moved to participate in the collaborative THM analysis and modeling of the FEBEX-DP experiment, a continuation/expansion of the THMC modeling conducted for the FEBEX-DP Project under the umbrella of the EBS task Force. Also, DOE proposed to the EBS Task Force leadership to include the HotBENT Column Test as a new modeling task (Section 3.3.2.3). This proposal was accepted as a new EBS Task 11, now led by LBNL researchers with seven participating modeling teams. As pointed out in Section 3.4.3 below, a few additional EBS tasks have recently been developed, which might also interest SFWST researchers.

An additional collaboration opportunity with SKB is dismantling the inner section of the Prototype Repository. The outer section of this field experiment was dismantled between November 2010 and December 2011, while the inner section continued to operate until recently. SKB decided in late 2022 to dismantle the inner section to understand the state of bentonite after more than 20 years of heating and hydration. SKB invited international collaborators, including DOE, to participate in the dismantling and data interpretation. SFWST is in discussion with SKB about a possible collaboration. See more information on the Prototype Repository Dismantling in Section 3.4.4.

3.4.2 GWFTS TASK FORCE

The main objective of the GWFTS Task Force is to develop and apply appropriate methods for investigating flow and transport in fractured crystalline rock to better understand the retention of radionuclides in crystalline rock and to improve the credibility of simulation models. The task force also provides a platform for interaction in conceptual and numerical modeling of groundwater flow and solute transport in fractured rock.

For the first few years of DOE's participation, the main modeling task conducted in the GWFTS task force was Task 8: Modeling of the BRIE at Äspö HRL. The BRIE experiment was a joint task shared between the GWFTS and the EBS Task Forces. The objective of the BRIE experiment was to enhance the understanding of the hydraulic interaction between the fractured crystalline rock at Äspö HRL and the unsaturated bentonite used as backfill. The experiment was subdivided into two parts: the first part involved the selection and characterization of a test site and two central boreholes, and the second part handled the installation, monitoring, and later overcoring of the bentonite-rock interface. Modeling groups, including a group of SFWST scientists, were able (a) to gain a better understanding of water exchange at the bentonite-rock interface and (b) to obtain better predictions of bentonite wetting in a fractured rock mass. Task 8 (BRIE) ended in FY17, and Task 9 was initiated, which involved modeling of two diffusion/sorption experiments: the Long-Term Diffusion Experiment at Äspö HRL and the REPRO (Rock Matrix Retention Properties) Experiment at Onkalo URL in Finland. Task 9 was concluded in 2021 with extensive discussion on the most important lessons learned.

A new Task 10 was introduced in 2020 and gradually became the only task the GWFTS worked on. The task title is "Validation Approaches for Groundwater Flow and Transport". The focus is on (1) improving our understanding of multi-scale flow channelization in fractured crystalline rock, and (2) validating fracture network models and other models that can account for such channelization. The spatial scales range from the small (within a single fracture) to the large (small fracture network) scale.

While previous GWFTS tasks typically involved experiments, the main interest in Task 10 is modeling methodologies and approaches, emphasizing validation and conceptual model uncertainty. Experiments are still needed, but in Task 10, they are used to assess validation strategies rather than the central element of the task. Figure 3.4-2 shows the structure of Task 10, starting in Task 10.1 with the development of a White Paper on pragmatic model validation methods, followed by testing of such methods at three different scales from single fracture to small network to block scale. As illustrated in Figure 3.4-3, HM laboratory experiments conducted on natural rock joints were included in Task 10.2 to examine validation approaches for flow within a single fracture with HM coupling.

In FY23, LANL researchers worked with other GWFTS task force team members to finalize the White Paper on DFN model validation as a framework document for model validation and as a reference planning document for the Task 10 validation activities. In parallel, LANL scientists developed capabilities to simulate channelized flow and transport in individual fractures and fracture networks. In past years, this work comprised initial simulations of transport in fractured rock, considering surface topography and textures with different connectivity structures. Recently, LANL's participation moved from Task 10.2 to Task 10.3, which focuses on the pragmatic validation of DFN models at the Small Network scale:

- Task 10.3.1 focuses on the Simple Fracture Network scale, limiting consideration to a single structure with a few intersecting features that can affect the pattern of flow and transport within the fracture.
- Task 10.3.2 considers the entire Discrete Fracture Network (DFN), including identified and statistically expected discrete fractures, at a Small Network scale of less than 100 m.

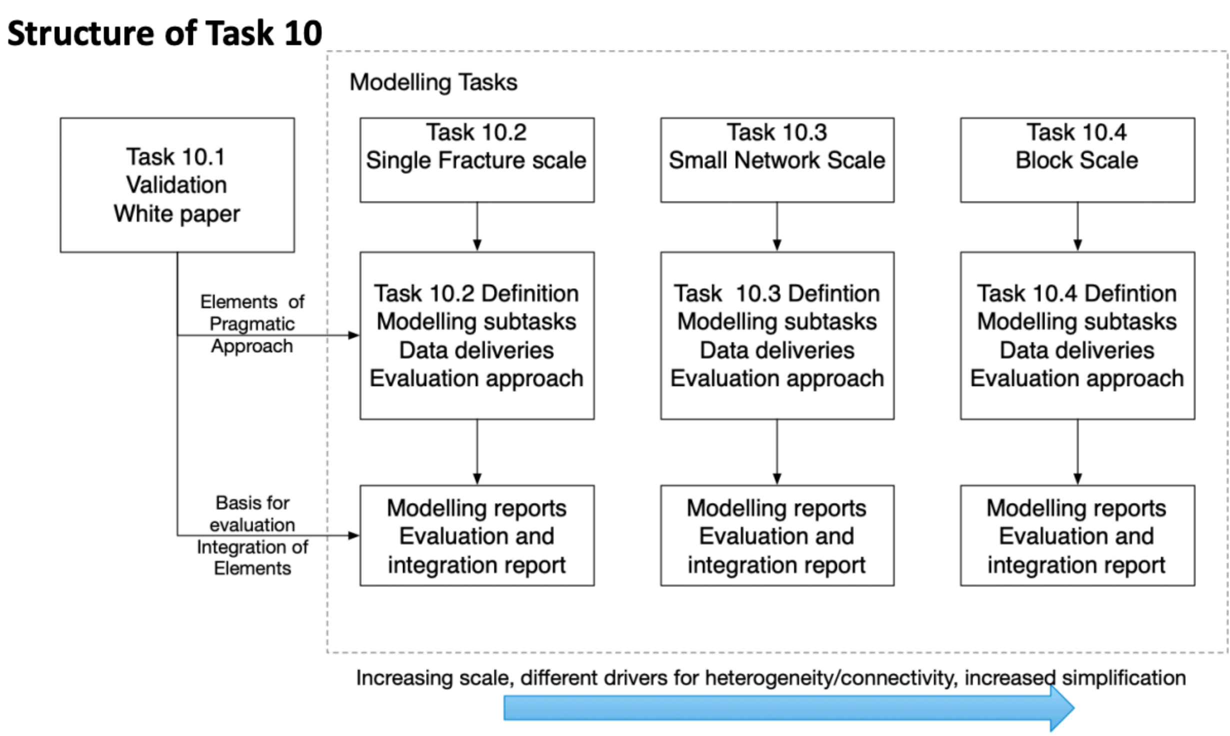

Figure 3.4-2. Structure of GWFTS Task 10 (Lanyon, 2021).

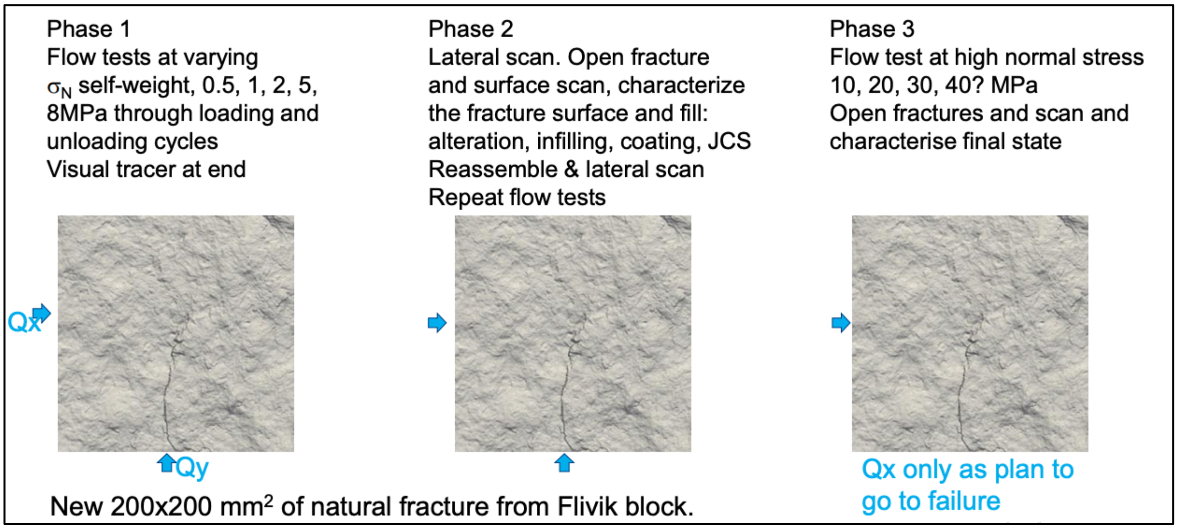

Figure 3.4-3. HM testing conducted for Task 10.2 (Bruines and Lanyon, 2021).

3.4.3 EBS TASK FORCE

As mentioned above, the EBS Task Force has historically involved two distinct focus areas, one on THM processes referred to as EBS-THM, and the other on chemical processes referred to as EBS-C. The two EBS sections on THM and C traditionally worked on different modeling tasks, and EBS Task Force meetings were jointly held but in separate sessions for THM and C. In recent years, activities of the EBS-THM and EBC-C focus areas have been more integrated.

- The main goal of the EBS-THM focus area is developing and applying general and effective tools for the advanced coupled THM 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 data, and (3) to evaluate the influence of parameter variations, parameter uncertainties, and model deficiency. Tasks in the EBS-THM Task Force did not have a fixed period but typically were finished in 4-5 years. New tasks were added when old tasks were finished and usually three to four tasks were running simultaneously. Tasks that were closed recently were Task 7 (Gas Transport in Bentonite), Task 9 (FEBEX *In-situ* Test), and Task 10 (Water Transport in Pellet Filled Slots). The currently active tasks are Task 11 (Berkeley High-Temperature Column Test, or HotBENT Lab #1 and #2), and Task 13 (Unsaturated Homogenization). SFWST scientists have actively participated in the EBS-THM focus area since FY19 and have primarily engaged in Tasks 9 and 11. Below, we briefly review the currently ongoing tasks in the EBS-THM Task Force, namely Tasks 11, and 13, and a new Task 14 that was added in FY24.
- The EBS-C focus area aims at advancing the fundamental understanding of physicochemical processes in clay or bentonite materials relevant to various aspects of safety assessment. In contrast to the EBS-THM section, which usually has a close connection between models and experiments, the “chemical” task force had been mainly working on conceptual model development and benchmark/modeling studies because of the complexity of conducting reactive transport modeling. After conducting a range of benchmark simulations and simplified modeling studies for several years, the EBS-C focus area decided in FY21 to (1) integrate the EBS-THM focus area, and (2) add lab and field monitoring data to its task portfolio. LBNL then proposed that the EBS-C focus area develop coupled THMC models for the FEBEX *in-situ* test, as part of

Task 9 in collaboration with the EBS-THM focus area. The proposal gained support initially as the teams participating in Task 9 proposed expanding their existing THM models to full THMC coupling. However, about two years after the task force accepted the proposal, LBNL was the only team conducting THMC simulations, while other teams did not make much progress. Ultimately, Task 9 ended in FY21. A new Task 12 was initiated in FY22 with a focus on modeling of physicochemical processes at the cement-bentonite interface. This task, led by LianGe Zheng from LBNL, is part of an integrated EBS Task Force portfolio. Both LBNL and SNL participate in the modeling work. Below, Task 12 is briefly described along with the other EBS-THM tasks.

3.4.3.1 BERKELEY HIGH-TEMPERATURE COLUMN TEST (TASK 11)

Task 11 involves the HotBENT Column Test (or HotBENT Lab #1) conducted at LBNL, a bench-scale experiment specifically designed to provide time-lapse CT and ERT images of THMC perturbation of a hydrating bentonite sample heated to a maximum temperature of 200 °C (Section 3.3.2.3). The task description was provided by LBNL and made available on the SKB task force website. Currently, three teams (LBNL, SKB, and Clay Technology) are modeling. In FY24, the new HotBENT Lab #2 test was added to Task 11. HotBENT Lab #2 and Lab #1 share the same configuration but have different bentonite properties and hydration pressure, which is ideal for sensitivity analyses. LBNL developed a THM model to interpret the data from the HotBENT Lab #1 test (Zheng et al., 2021; 2022). The THM model reasonably matches the CT density data and qualitatively matches the displacement data (Yoon et al., 2024). Future work will refine the model to explain the dynamic interaction between hydration and swelling/compaction. SKB finished a 1D model using the Comsol Multiphysics software, starting with a TH model in 2023, which then evolved into a THM model in 2024. SKB also modeled the HotBENT Lab #2. Clay Technology developed a 2D THM model for HotBENT Lab #1 and provided a decent match of the temperature and density data. They plan to simulate HotBENT Lab #2 in the future.

3.4.3.2 CEMENT-BENTONITE INTERACTION (TASK 12)

In Task 12, modeling teams collaboratively simulate long-term reactions occurring at cement-bentonite interfacial regions about time-dependent mineralogical, chemical, or textural changes. Details on how these reactions occur in space and time define whether an aged cement/bentonite interface may impede radionuclide transport (a beneficial effect) or cause delays in bentonite saturation (an unwanted effect). Teams started with three modeling benchmark cases for different types of bentonite, cement, temperature (non-isothermal versus isothermal), and saturation conditions (unsaturated in bentonite versus saturated). Teams will later move to simulate relevant experiments. Data from the CI-D project at Mont Terri may be used for this purpose (Section 3.1.4). Considering the limit of continuum scale reactive transport model to describe the change in pore structure and the resulting permeability change, LBNL scientists in FY21 and FY22 attempted to use a pore-to mesoscale model based on the Lattice Boltzmann Model (LBM) approach to simulate the cement-bentonite interface area. LBM may be suitable to describe the change in pore structure and the resulting permeability change with a feasible computation load for a scale of 10-20 cm. After completing the preliminary model studies, it became clear, however, that the LBM model is too computationally expensive to simulate a spatial scale of 20 cm for 100,000 years. To align with other international teams in Task 12, the LBNL team re-focused on the benchmark problem using a continuum-scale model in FY23.

Task 12 was divided into three subtasks to simulate different initial saturation states of bentonite and types of concrete. Subtask A is conducted to study the interaction between MX-80 and Ordinary Portland Cement (OPC); Subtask B focuses on the interaction between MX-80 and low pH OPC; Subtask C is like Subtask A, but has a different initial hydraulic condition. Benchmarking a reactive transport modeling for the concrete/bentonite interaction is very challenging because many aspects of the model development are still being determined, including thermodynamic database, kinetic reaction rate, selection of aqueous complexes, and choice of secondary minerals. The modeling teams including LBNL, SNL, SKB, and SURAO met regularly online to determine modeling details. Because of different ways of establishing initial porewater concentrations expanded Subtasks A and B to Subtasks A1, A2, and A3, and Subtasks B1, B2, and B3.

The LBNL team finished simulations for Subtasks A and B (see Section 6.2.5 in this report, and for more detailed information, see Section 7 of Zheng et al., 2024). The SNL team developed and applied a 1D reactive transport model for Subtasks A, B, and C (see Section 6.2.5 in this report, and for more detailed information see Section 4 of Jové-Colón and Lopez, 2024). The SKB team finished Subtasks A, B, and C and the SURAO team finished Subtasks A and B. A systematic comparison of Subtask A between model results of LBNL, SNL, SKB, and SURAO was given by LianGe Zheng in Task Force Meeting #36 in April 2024 in Prague, Czech Republic. Despite the differences in some aspects of the model setup, such as reaction rate and diffusion coefficient, all the models are qualitatively consistent in mineral dissolution and precipitation. LBNL and SNL models predict a broader impacted area around the interface. In contrast, SKB and SURAO models suggest that the area affected by dissolution and precipitation is constrained to a few centimeters around the interface.

3.4.3.3 UNSATURATED HOMOGENIZATION (TASK 13)

This task involves a series of laboratory tests on bentonite homogenization conducted by CIEMAT (Villar et al., 2020). The question asked is to which extent bentonite would be capable of swelling into a gap or void and, if so, what the resulting bentonite properties would be. In this test program, FEBEX bentonite samples were compacted inside stainless steel rings, and a gap was left at the top. The granulated bentonite was initially compacted with its hygroscopic water content (14%) at a target dry density of 1.7 g/cm^3. These samples were hydrated and later dismantled after different periods. The final water content and dry density of the bentonite at different levels of the sample were measured, as well as the incremental bentonite intrusion into the gap (see example results in Figure 3.4-4) and the resulting pore size distribution. The hydration experiments were conducted as part of a European Union Project called BEACON, which aimed at developing and testing the tools necessary to assess the mechanical evolution of a bentonite barrier and the resulting sealing ability of the barrier.

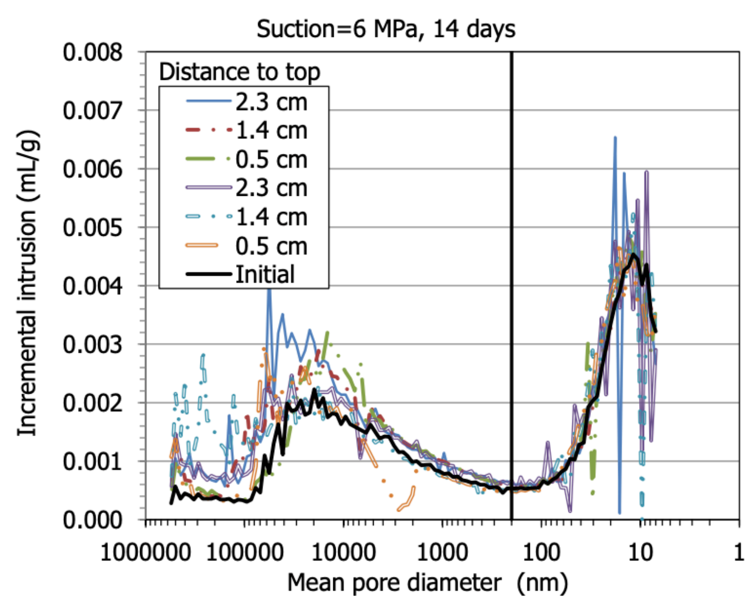

Figure 3.4-4. Incremental intrusion of pelleted bentonite swelling into a gap (Gens, 2021).

Activities under Task 13 started in 2021; CRIEPI (Japan), BGE (Germany), Clay Tech (supported by SKB), and Institute of Genomics (supported by SURAO) are the participants of this task. SFWST participation is not currently considered. A synthesis of model results was given in Task Force Meeting #36 in April 2024 in Prague, Czech Republic.

3.4.3.4 SLOW HYDRATION OF BENTONITE (TASK 14)

The hydration of the bentonite buffer in argillite or granite host rock depends on the ability of bentonite to draw water from the host rock (based on the capillary pressure gradient between the bentonite and rock) and the ability of the host rock to supply water. For a host rock with low permeability and less mobile water, the water supply can limit how fast the bentonite buffer becomes saturated. This task, therefore, focuses on simulating a scenario with a limited water supply from the host rock. It involves modeling a laboratory column test conducted at BGR (Task 14A) and the HE-E heater test conducted at Mont Terri (Task 14B). The result of laboratory testing will be used to design cases with a limited water supply to the bentonite. The HE-E heater test demonstrated that even after eight years of heating, the bentonite area near the heater remained at a low water content, and hydration progressed very slowly. Task 14 will provide an opportunity to study the hydration of bentonite under a limited water supply from host rock and tackle the issue of upscaling from laboratory to field experiments. Task 14 was formally introduced into the EBS Task Force in 2024. Detailed experimental plans in Task 14A were presented in Task Force Meeting #36. BGR, CRIEPI, and Clay Technology are interested organizations and modeling teams. SFWST will evaluate the benefits and resources to see if DOE wants to join this new task.

3.4.4 RETRIEVAL OF THE INNER SECTION OF THE PROTOTYPE REPOSITORY

The Prototype Repository field test is a long-running demonstration experiment that was constructed in the early 2000s at the Äspö HRL at a depth of 450 m. The test was designed to simulate the KBS-3 repository concept consisting of canisters with electric heaters, bentonite buffer, and backfill. The test consisted of two sections: an outer consisting of two deposition holes and an inner with four deposition holes (Figure 3.4-5). The two sections were separated by a concrete plug that allowed the two sections to be dismantled at different times. The outer section was dismantled between November 2010 and December 2011, while the inner section continued to operate. In late 2022, SKB decided to dismantle the inner section to understand the state of bentonite after more than 20 years of heating and hydration.

SKB invited international partners to join the project “Retrieval of the Inner Section of the Prototype Repository.” Scientists from SFWST met a few times with SKB in early 2023 to get clarity about the benefits and costs of joining the project as a research collaborator. After careful evaluation, Prototype Repository appears to be substantially different from the full-scale FEBEX heater test and will provide a chance to study a different type of bentonite (Wyoming-type bentonite) under extended long-time hydration and heating conditions. This will improve the campaign’s understanding of the long-term alteration of bentonite. LBNL, SNL, and LANL provided a list of preliminary research ideas to SKB (Table 3.4-1). SKB has expressed interest in these research ideas and prepared a draft contract for DOE. Currently, DOE is reviewing the contract.

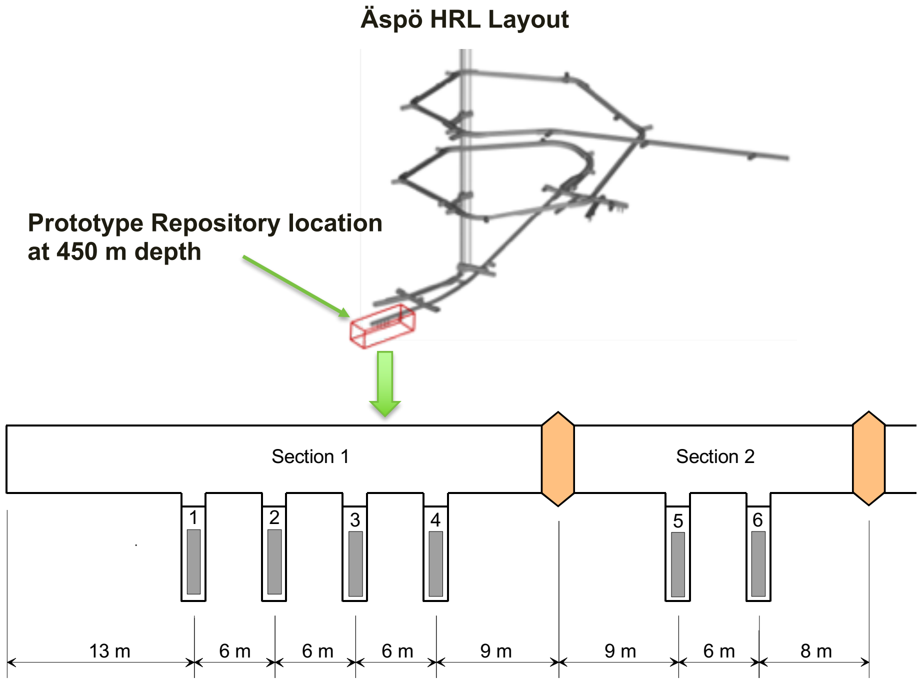

Figure 3.4-5. Äspö HRL layout and configuration of the Prototype Repository test (modified from Svemar et al., 2016).

Table 3.4-1. Preliminary experimental ideas of using samples retrieved from the dismantling of the Prototype Repository.

DOE Lab	Proposed R&D Activity	Description
LBNL	Study on the sorption capacity and diffusivity of bentonite sample after long-term heating and hydration	Batch sorption tests using bentonite retrieved from heater test and original material in solution containing radionuclide (e.g., U). Through-diffusion test will be conducted for both retrieved and original bentonite samples
LBNL	Study bentonite swelling characteristics after long-term heating and hydration	μ-oedometer system will be used to measure bentonite swelling characteristics
LBNL	Study the biological characteristics of bentonite sample after long-term heating and hydration	DNA extraction will be conducted for a series of samples collected at different locations and original material
SNL	Understanding structural homogenization of compacted bentonite blocks and gap-filling pellets during hydration	Intact core samples will be carefully retrieved. The samples and materials will then be characterized using optical microscope, CT-scanning, XRF, and XRD
SNL	Understanding metal corrosion at copper-bentonite interface	The metal surface and the interface of copper-bentonite will be examined using multiple microanalytical techniques (e.g., optical microscope, SEM, AFM and XRD)
LANL	Comprehensive mineral phase characterization and crystal chemistry of bentonite	Work with both LBNL and SNL to provide full mineral characterization and crystal chemistry of shared samples
LANL	Copper corrosion in bentonite clay environment	Coordinate with SNL to establish bulk chemistry mass balances at the interface based on observed mineralization

3.4.5 SUMMARY OF INTERNATIONAL COLLABORATION INITIATIVES ORGANIZED BY SKB

Collaboration with SKB has primarily centered on the SKB Task Forces in the past, but the planned dismantling of the Prototype Repository provides another valuable opportunity for collaboration.

Benefits of Participation in the SKB Task Force:

- Access to several sets of experimental data from URLs in crystalline rock.
- Opportunity to perform modeling and analysis of existing field and laboratory data in collaboration with other modeling groups (typically less direct interaction with the project teams that run or interpret the experiments).
- Performing simulations for benchmark problems to improve conceptual understanding and test modeling capabilities.

Potential Benefits of Participation in the "Retrieval of the Inner Section of the Prototype Repository Prototype Repository" Project:

- Fill in the knowledge gap about bentonite alteration. Geochemical alteration of bentonite after long-term heating and hydration has been a critical issue for the safety of geologic repositories. Participation in the Prototype Repository provides a unique opportunity to study bentonite alteration under long-term hydration and relatively low-temperature heating (50-80°C) in contrast to the FEBEX-DP (100°C) and HotBENT (200°C).
- Gain insight into using large-scale field tests and underground research laboratories to support license application.

Status of Participation:

DOE joined both SKB Task Forces in January 2014. Under the GWFTS Task Force umbrella, SFWST researchers finalized their involvement in GWFTS Task 9 (diffusion and sorption experiments). Subsequently, they worked on Task 10, which focuses on flow channelization in fractured crystalline rocks and validation of DFN models (Section 3.4.2.1). Regarding the EBS Task Force, the HotBENT Column Test series conducted at LBNL was brought into the Task Force as Task 11: SFWST researchers not only provided the test details and all the data needed for the model but also contributed with advanced THM models (Section 3.4.3.1). LianGe Zheng from LBNL is chairing Task 12 (Cement-Bentonite Interaction) and both LBNL and SNL have been progressing in developing reactive transport models for this task (Section 3.4.3.2).

Outlook:

SFWST's participation in the SKB task forces is currently focused on Task 10 in the GWFTS Task Force, and Tasks 11 and 12 in the EBS Task Force. The SFWST campaign has assumed more responsibility for task selection and leadership in these tasks. In Task 11, it was the first time a laboratory experiment conducted by SFWST has been used for a Task Force modeling effort; in Task 12, it was the first time an SFWST scientist chaired a task. Having multiple international teams contribute to the interpretative modeling of the high-temperature column test is a win-win for SFWST and its international partners, and leading a task will help SFWST to use international collaboration to further improve R&D in SFWST. The SKB EBS Task Force has added a new Task 14; SFWST will evaluate the task and decide based on SFWST priorities.

SFWST is engaged in discussions with SKB about joining the “Retrieval of the Inner Section of the Prototype Repository” project. SKB International provided a draft contract, which DOE is reviewing.

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Antonio Gens, EBS Task Force for THM, from UPC, Spain
Patrik Sellin, Point of Contact for Prototype Repository

3.5 NEA'S COOPERATIVE INITIATIVES

Here we briefly touch on selected collaboration initiatives provided by the NEA. As opposed to the previous Sections 3.1 through 3.4 that describe active research opportunities associated with international URLs, the nature of the engagement with NEA is typically less focused on active collaboration rather than on the exchange of information and the development of shared approaches or databases. There is one exception: The Horonobe International Project, organized under the umbrella of NEA and introduced in Section 3.5.7 below, comprises international joint experiments and related analysis at the Horonobe URL in Japan.

3.5.1 NEA'S INTEGRATION GROUP FOR THE SAFETY CASE (IGSC)

The Integration Group for the Safety Case (IGSC) is the main technical advisory body to NEA's Radioactive Waste Management Committee (RWMC) on deep geological disposal, particularly for long-lived and high-level radioactive waste. It was established in 2000 to recognize the need to foster full integration of all aspects of the safety case. The mission of the IGSC is to assist member countries in developing effective safety cases supported by a robust scientific-technical basis. In addition to the technical aspects in all developmental stages of repository implementation, the group also provides a platform for international dialogues between safety experts to address strategic and policy aspects of repository development. Member countries are from Belgium, Canada, Czech Republic, Finland, France, Germany, Hungary, Japan, Korea, Netherlands, Russia, Spain, Sweden, Switzerland, United Kingdom, USA, European Commission, and IAEA. US participants are the DOE, NRC, EPA, and the NWTRB.

To help accomplish its activities, the IGSC is supported by four subgroups carrying out tasks on specific topics. Three subgroups that focus on the feasibility of repositories in three different generic host rock types are described below: Clay Club, Salt Club and Crystalline Club. A fourth subgroup, the Expert Group on Operational Safety (EGOS), deals with the operational safety of geological repositories.

Projects of the IGSC are critical for coordinating international R&D programs to share experience, develop consensus on state of the art, and create an understanding of specific topics and technical tools to support the safety case. Since the development of a safety case involves inputs from various disciplines (e.g., engineering, geology, radiological protection, etc.), IGSC activities are organized in the following thematic framework to foster consensus on best practices and advance the development of innovative approaches used in all stages of repository implementation: (1) Scientific basis, (2) Safety assessment strategy and tools, (3) repository design and implementation, and (4) Data information and management. The IGSC also participates in international projects and work activities to stay abreast of state-of-the-art knowledge and technologies in safe radioactive waste management. Examples of international projects include, but are not limited to, Fate of Repository Gases (FORGE) and the European Joint Program on Radioactive Waste Management (EURAD).

3.5.2 NEA'S CLAY CLUB

In 1991, the 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." Since 2000, the Clay Club has operated under the umbrella of NEA's IGSC, an international forum on confidence building in repository technical safety cases and on the underlying methodological and scientific bases for 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 and provides advice to the IGSC on major and emerging issues related to the knowledge of the multi-scale characterization, numerical model simulation, and barrier performance of argillaceous media. In particular, the Clay Club addresses recommendations, trends, and information gaps concerning issues such as:

- Improving current knowledge regarding the long-term barrier integrity of argillaceous rock as relevant to establishing a deep geological repository safety case on time frames of one million years,
- Developing best international practice concerning multi-disciplinary laboratory, borehole and *in-situ* characterization of argillaceous sediments necessary to understand far-field phenomena governing repository evolution, behavior and long-term performance, and
- Refining the understanding of repository-induced effects in argillaceous rocks during excavation, operation, and post-closure phases.

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 work topics reflect issues of common interest, considering the experience, progress, and challenges of national programs. Decisions on projects are made on a consensus basis, thereby considering the importance and urgency of the issue, the breadth of interest (i.e., the number of national programs for whom the issue is regarded as 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.

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. The Clay Club comprises 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 R&D institutions. Each member organization sends a representative to the annual meetings and provides a report on ongoing activities. Clay Club members are expected to: (1) promote Clay Club activities in their own organization; (2) provide relevant data and bibliographic material to support Clay Club initiatives; and (3) make human or financial resources available to the Clay Club initiatives as appropriate and on an ad hoc basis.

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 club members are institutions from Belgium, Canada, France, Germany, Hungary, Japan, Netherlands, Spain, Switzerland, the United Kingdom, and the USA. Michelle Plampin (USGS) and LianGe Zheng (LBNL) are the U.S. representatives. The Clay Club held its latest #33 meeting in September 2023. In the meeting, the NEA Secretary of the Radioactive Waste Management Committee briefly updated the status of the eight technical committees (including the environmental aspects of which the Clay Club is part), optimization aspects, integrated management aspects, regulation aspects, social aspects, economics aspects, and legal aspects. The NEA thermochemical database (TDB) project also gave a status update.

The Clay Club also conducts or commissions detailed studies on relevant topics. Currently, the club is wrapping up the "ClayWat Project" (Mazurek et al., 2020), which studies porewater mobility and binding state in argillaceous rocks. The final report (Mazurek et al., 2023) was released in May 2023 and discussed in the #33 meeting. This report focuses on characterizing the pore-space architecture and examining how pore-water molecules interact with the immediate vicinity of clay surfaces. A total of 12 samples were collected through the Clay Club membership, sourced from formations being studied as potential host rocks for radioactive waste disposal or from underground research laboratories in clay-rich environments. Another project, initiated in 2020, seeks to analyze anomalous pore water pressures in shale formations. However, the project has been delayed due to some contracting issues, and thus, no research work has been conducted to date.

3.5.3 NEA'S SALT CLUB

The "Salt Club" (also known as "Expert Group on Repositories in Rock Salt Formations") brings together nations currently considering rock salt as a candidate medium for deep geologic disposal of High-Level Waste (HLW) and long-lived radioactive waste. The club aims 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 scientific aspects, the working group also aims at transferring programmatic and technical knowledge to younger staff and 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 comprises 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. The U.S. DOE is a current member of the Salt Club; Kris Kuhlman (SNL) has chaired the Salt Club since January 2021. Other members are from Germany, the Netherlands, Poland, Romania, the United Kingdom and Australia.

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; since then, the members have met roughly once a year. The Salt Club has the following areas of interest:

- Geomechanical issues (coupled processes, EDZ behavior, rock mechanic issues, backfilling, sealing and plugging of rooms, drifts, and 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;
- Compiling databases of relevant salt physical properties from countries around the world;
- Contributions to the Safety Case (e.g., FEP catalog, scenarios, performance assessment issues, uncertainties, use of natural analogs); and
- Lessons learned from failure events/processes of conventional salt mines.

In FY24, SFWST researchers continued their involvement in the NEA Salt Club activities. A Salt Club working group on scenario development includes US, German, UK, and Dutch colleagues. This group continues progressing on an NEA Salt Club report on scenario development, which will be submitted to NEA in late 2024. A small group from this working group has finished a journal manuscript on the topic (Kuhlman et al., 2024b). The group presented its status at the in-person NEA Salt Club meeting in Manchester, UK, in June 2024.

3.5.4 NEA'S CRYSTALLINE CLUB

The "Crystalline Club" (also known as "Expert Group on Geological Repositories in Crystalline Rock Formations") was added to the portfolio of NEA's radioactive waste disposal working groups in 2017. Recognizing the mutual benefits of joint international research efforts and the successes of the NEA Clay Club and Salt Club, delegates from the Czech Republic, Germany, Japan, Russian Federation, Spain, Romania, Switzerland, and the United States requested that the NEA establish a similar group for the study of crystalline rocks. Among the different geological formations considered suitable for hosting geological repositories, crystalline rocks are characterized by high strength, providing cavity stability, low heat sensitivity, permeability, and dissolution properties. Because fractures are common in crystalline rocks and tend to enhance groundwater transport of radionuclides, t engineered barriers such as waste containment and bentonite backfill have added importance. Although an advanced scientific and geotechnical understanding of crystalline rocks has been accumulated by the dedicated research carried out by several countries, there are research areas in which member countries may benefit from knowledge exchange, in-depth discussions, and joint R&D efforts.

The work program and modus operandi of the Crystalline Club are coordinated by a Crystalline Club Bureau, which consists of one expert from each member country. Project topics are driven by common interests among members. The mode of cooperation is by plenary meetings, periodic general workshops, and electronic media. Over the past year, the club has conducted a global literature review to identify chemical processes potentially critical to crystalline repository performance, including effects on canister performance. The review will produce an organized electronic database of the results and a report summarizing the findings. Currently, the Crystalline Club has 11 "member countries": the U.S., Finland, Korea, Canada, Czech Republic, Romania, Germany, Japan, Russia, Spain, and Switzerland. Paul Mariner of SNL, nominated by DOE to participate in the Crystalline Club, is one of the club's vice chairs.

3.5.5 NEA'S THERMOCHEMICAL DATABASE PROJECT (TBD)

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, the Czech Republic, Finland, France, Germany, Japan, Spain, Sweden, Switzerland, the United Kingdom, and the United States. A 2015 report on the history of NEA TDB activities summarizes the project's accomplishments since its inception in 1984 (Ragoussi and Brassinnes, 2015). DOE has been participating in the TDB Project since its inception. Mavrik Zavarin of LLNL is the U.S. NEA-TDB Management Board and Executive Group representative. The close engagement with the NEA TBD Project ensures that the generic disposal system modeling conducted by SFWST researchers is aligned with internationally accepted practices for repository performance assessment calculations.

The TDB project has operated in six phases over almost two decades. During the initial phases of the project, a high priority was assigned to the critical evaluation of the data of inorganic compounds and complexes of the actinide's uranium, americium, neptunium, and plutonium, as well as the inorganic compounds and complexes of technetium. The second phase supported radioactive waste management programs by updating the existing database and applying the TDB methodology to new elements in radioactive waste (as fission or activation products): nickel, selenium, zirconium, and 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 to prepare guidelines for evaluating thermodynamic data for solid solutions. The fourth phase (2008-2014) started the second portion of the iron review (Part 2), a review of molybdenum, and a review of auxiliary data, which includes species and compounds necessary to describe the aqueous chemistry of aluminum and silicon, data on inorganic species and compounds of elements such as iodine, boron, magnesium, calcium, strontium, and barium. Phase V of the NEA-TDB program, conducted from 2014-2019, took on a second update to actinide and fission product volumes and two State-of-the-Art reviews--Cement Minerals and High Ionic Strength Aqueous Systems. Phase VI of the NEA-TDB is the current phase and is projected to end in 2024.

NEA-TBD is currently discussing options for continuing the TDB effort into Phase VII. There is an overwhelming consensus that the NEA-TDB project remains an important asset to the international nuclear waste research community. Phase VII is projected to start in early 2025 if all participating member parties have signed the Framework Agreement. We anticipate that the U.S. will continue to participate as a member of the NEA-TDB. Phase VII activities will include an update to radionuclide complexation with organic complexants and a review of the state-of-the-art regarding temperature and pressure dependence of radionuclide speciation and solubility. Phase VII will also allow participating countries to propose initiating new activities within the scope of the NEA-TDB mission.

FY24 activities conducted by SFWST scientists in support of the NEA-TDB project are summarized in Section 6.9.3. A continuing focus has been to support the U.S. participation in the NEA TDB Project and develop mechanisms for integration of NEA-TDB thermochemical data with LLNL's SUPCRTNE thermodynamic database. FY24 efforts also ensured interoperable database development across multiple international database development activities. For more detailed information, see FY24 reports by Zavarin et al. (2024a,b).

3.5.6 NEA'S INFORMATION, DATA, AND KNOWLEDGE MANAGEMENT GROUP (IDKM)

NEA's RWMC continues to demonstrate commitment in the data sciences area. In 2019, the RWMC created a working group dedicated to Information, Data and Knowledge Management (IDKM) in the radioactive waste management field. This group extends the objectives of the previous activities to holistically cover all waste management phases from cradle to grave while preserving the awareness of disposed wastes and repositories for future generations (McMahon, 2019; NEA, 2019a,b,c).

Four IDKM plenary meetings have been held since 2019 in the NEA offices at Boulogne-Billancourt, France. The first of these plenary meetings was the official kick-off meeting for IKDM, held virtually on September 15-17, 2020, with 42 representatives from 12 NEA member countries and the European Union (EU). Subsequent plenary meetings included annual progress updates by the four individual working groups and discussions of future activities. Programs of Work (POW) for the IDKM and the four working groups it oversees are updated annually and formally approved at each IDKM plenary meeting. DOE is represented by Chris Camphouse (SNL) on the IDKM Governing Bureau. Janette Meacham (SNL) represents the DOE on the Governing Bureau of the Knowledge Management subgroup.

3.5.7 HORONOBE REPOSITORY PROJECT (HIP)

The Horonobe International Project (HIP) is an international Joint Project organized under the umbrella of the NEA with the main theme of tackling "Challenges for Developing Advanced Technologies and Human Resources Towards Long-Term Implementation of Geological Disposal". HIP involves joint research associated with field characterization and experiments conducted at JAEA's Horonobe URL, located in a sedimentary (mudstone) formation up to 500 m deep below the island of Hokkaido in Japan (Figure 3.5-1). Eleven organizations from eight countries came together for the first HIP Management Board meeting in April 2023 and soon after launched participating the project. The US program is currently not engaged with HIP.

The Project is organized in two main phases: 2023-2025 and 2025-2029. The main objectives of the HIP are to:

- Develop and demonstrate advanced technologies to be used in repository design, operation and closure, and a realistic safety assessment in deep geological disposal; and
- Encourage and train the next generation of engineers and researchers by sharing and transferring a vast amount of knowledge and experience developed to date in relevant organizations worldwide.

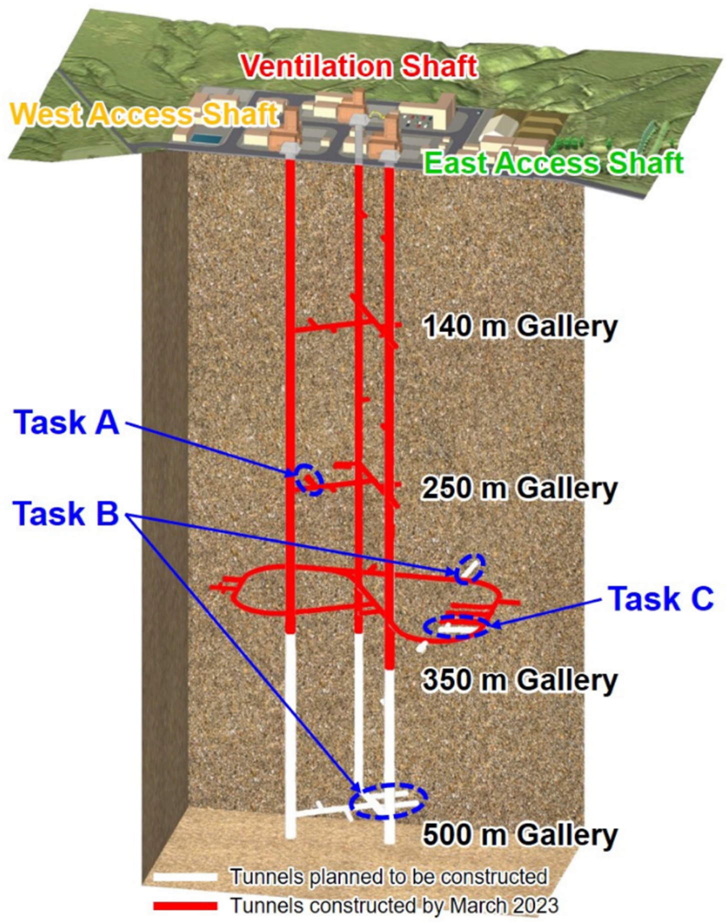


Figure 3.5-1. 3D schematic of the Horonobe URL in Japan.

There are currently three HIP projects:

- **Task A - Solute Transport Experiment with Model Testing**

  Attempts have been made to enhance the technical reliability of solute transport models for repository safety assessments by *in-situ* tracer tests. In general, the results of tracer tests are often modeled to produce a set of 'best fit' values for the transport parameters by comparing calibrated model curves with the experimental breakthrough curves. Still, the modeled values are not always a unique solution. This could be because the actual structures and processes relevant to solute transport are unknown. Hence, these are represented in the solute transport models with effective parameters in a relatively straightforward manner. It is thus suggested in Task A that detailed, realistic information on the relevant structures and processes should be obtained through a series of tracer tests and the subsequent rock characterization under *in-situ* conditions at HIP (Figure 3.5-2). This would allow the models and model assumptions to be rigorously tested and their technical reliability considerably enhanced. This task aims to develop more realistic 3D solute transport models that can be applied to perform a repository safety assessment for fractured-porous sedimentary rocks.

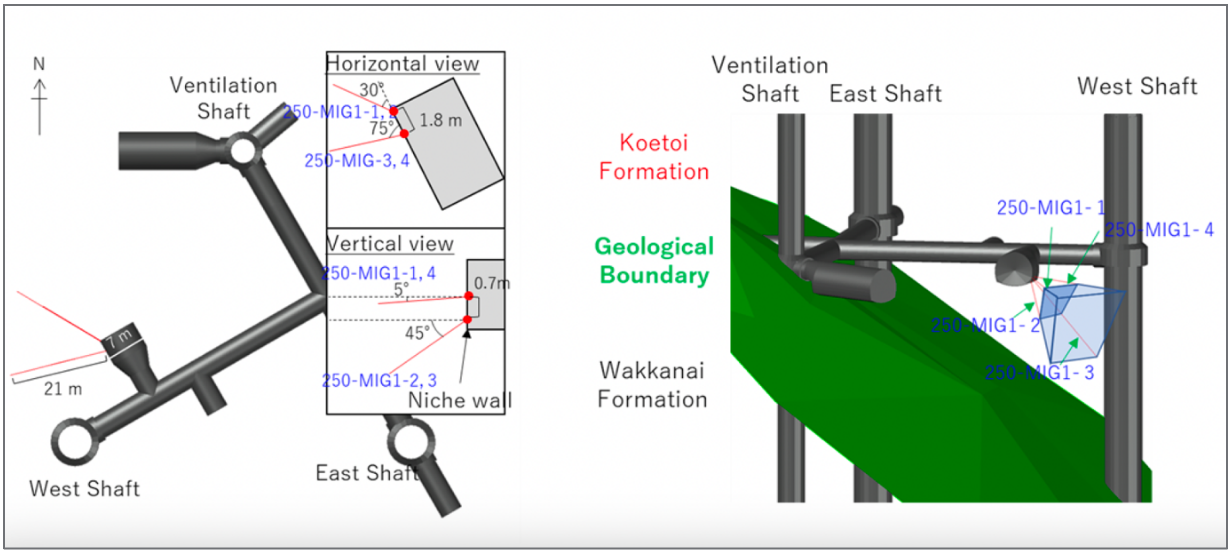


Figure 3.5-2. Layout of the four boreholes for the tracer experiments planned at the 250 m Gallery.

- **Task B – Systematic Integration of Repository Technology Options**

To arrange and construct disposal tunnels and pits or holes in suitable rock volumes, it is of great importance to design the detailed layout of them taking into consideration the distribution, spatial scale and hydraulic properties of faults and fractures and their potential impacts on likely radionuclide migration and the long-term stability of EBS. Criteria are thus required for locating the disposal tunnels and pits or holes and their adequacy should be ensured through the demonstration of a workflow from initial geological characterization to the design and construction of a tunnel and deposition holes (Figure 3.5-3). As a range of technology options for each process have been developed to date, such options should be advanced using the state-of-the-art technology as possible and the systematic integration of available options should then be demonstrated. The main aims of this task are to: (1) Develop technology options that could contribute to the operation of disposal sites, (2) Establish the concepts and criteria for locating disposal pits or holes in suitable rock domains around the disposal tunnels, and (3) Demonstrate the systematic integration of available technology options to arrange and construct the disposal pits or holes.

- **Task C – Full-Scale EBS Dismantling Experiment**

It is important to evaluate the evolution of near-field THMC conditions over time during the transition period following the emplacement of waste forms. This is because such information would allow the near-field initial conditions to be defined for safety assessments and the overpack lifetime to be predicted. To this end, the full-scale EBS performance experiment for vertical EBS emplacement has been carried out at the 350 meters Gallery since 2014, with the aims of understanding the THMC coupled processes and testing the THMC coupled simulation code during backfilling the EBS and tunnel and its subsequent dismantling (see also Section 3.2.2.4 for the related DECOVALEX-2019 task and Figure 3.2-6 for a schematic depiction of the EBS experiment). The previously installed sensors have obtained the many relevant measurements. However, as the information available from the sensors would not allow the conditions and processes occurring at the interfaces of the different EBS materials to be understood in detail, the experimental setup is dismantled to acquire more detailed information. The main aim of this task is to test THMC coupled simulation codes rigorously by understanding the near-field THMC coupled processes in more detail.

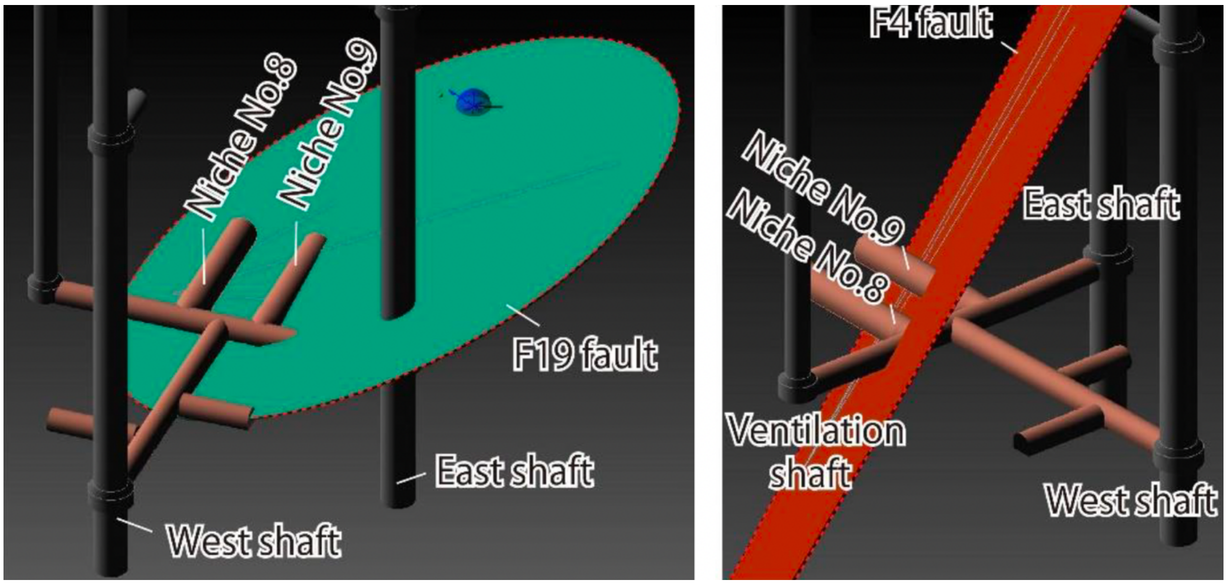


Figure 3.5-3. Predicted fractures in and around the 500 m Niches No. 8 and No. 9.

3.6 EUROPEAN UNION RESEARCH PROGRAMS

The European Union supports substantial long-term research and innovation programs, including EURAD, which stands for "European Joint Program on Radioactive Waste Management". A new five-year EURAD program, referred to as EURAD-2, has been in planning and development over the past few years; the program officially commences in October 2024. To conduct this program, EURAD-2 gathers (1) waste management organizations (WMOs) having the ultimate responsibility for the implementation of geological disposal, (2) technical support organizations (TSOs) carrying out activities aimed at providing the technical and scientific basis for supporting the work and decisions made by a national regulatory body, and (3) research entities (REs) working to different degrees on the challenges of radioactive waste management including disposal (and sometime in direct support to implementers or WMOs or TSOs). The program aims to ensure cutting-edge knowledge creation and preservation in view of delivering safe, sustainable and publicly acceptable solutions for the management of radioactive waste across Europe now and in the future.

At the beginning of the planning process for EURAD-2, European Union representatives reached out directly to SFWST leadership to advocate for synergistic collaboration between EURAD-2 work packages and selected SFWST activities. In response, the SFWST program evaluated technical alignment with the emerging EURAD-2 work packages and mapped technical contact points to those work packages where collaboration was deemed most beneficial. In FY23 and early FY24, the SFWST technical contact points for these work packages started interacting with their EURAD-2 counterparts to discuss possible collaboration and plan joint activities. At the end of this process, some of DOE's national laboratories (e.g., LBNL, SNL, LLNL, ORNL, PNNL) were incorporated as so-called Associated Partners into selected work package proposals for EURAD-2. The planned mode of operation is that these five labs above are not funded out of EURAD-2. Rather, they are getting their funding for EURAD-2 participation as part of their ongoing work in related SFWST work packages.

In April 2024, the proposal for EURAD-2 was accepted by the European Commission and grant/consortium agreements were finalized a few months later. A kick-off meeting planned for October 23-24, 2024, in Ghent, Belgium, will officially launch the program. Table 3.6-1 lists all EURAD-2 work packages with SFWST participation and points of contact on both sides. Work packages are either Research Projects (typically five years) or Strategic Studies (typically two years). SFWST selected nine work packages, seven Research Projects and two Strategic Projects. The SFWST points of contact for these work packages will interface with EURAD-2 through quarterly meetings (virtual), annual meetings (in-person), and joint reports (via extraction of information from our milestones). They will communicate the SFWST campaign activities to EURAD-2 and will inform the campaign about the activities performed in the nine work packages. This will guide annual planning of work on both sides to leverage activities and/or refine approaches in particularly related areas.

Table 3.6-1. EURAD-2 work packages with SFWST participation.

EURAD-2 WPs	Short Title	Type	EURAD-2 WP Leader	DOE SFWST TPOC - Primary	DOE SFWST TPOC - Supporting
WP1: ASTRA	Alternative RWM STRAtegies	Strategic	Marja Vuorio (COVRA) marja.vuorio@covra.nl	Tara LaForce (SNL) tlaforc@sandia.gov	Dave Sassani (SNL) dsassan@sandia.gov
WP3: FORSAFF	Waste Management for SMRs and Future Fuels	Strategic	Timothy Schatz (VTT) timothy.schatz@vtt.fi	Ed Matteo (SNL) enmatte@sandia.gov	Scott Sanborn (SNL) sesanbo@sandia.gov
WP8: SAREC	Release of spent fuel	Research	Olivia Roth (SKB) olivia.roth@skb.se	Brady Hanson (PNNL) brady.hanson@pnnl.gov	Jeff Fortner (ORNL) fortnerja@ornl.gov
WP9: InCoManD	Containers/canisters	Research	Aurelien Debelle (Andra) aurelien.debelle@andra.fr	Yifeng Wang (SNL) ywang@sandia.gov	Charles Bryan (SNL) crbryan@sandia.gov
WP10: ANCHORS	Bentonite/buffer/backfills	Research	Nadia Mokni (IRSN) nadia.mokni@irsn.fr	LianGe Zheng (LBNL) LZheng@lbl.gov	Ed Matteo (SNL) enmatte@sandia.gov
WP13: RAMPEC	Radionuclide mobility under perturbed conditions	Research	Marcus Altmaier marcus.altmaier@kit.edu	LianGe Zheng (LBNL) LZheng@lbl.gov	Carlos Jove-Colon (SNL) cfjovec@sandia.gov
WP16: HERMES	High-fidelity simulations for strongly coupled processes	Research	Sergey Churakov (PSI) sergey.churakov@psi.ch	Paul Mariner (SNL) pmarine@sandia.gov	LianGe Zheng (LBNL) LZheng@lbl.gov
WP17: CFSD	Criticality safety	Research	Madalina Wittel (nagra) Madalina.wittel@nagra.ch	Laura Price (SNL) llprice@sandia.gov	Justin Clarity (PNNL) justin.clarity@pnnl.gov
WP18: DITUSC	Thermodynamic database	Strategic	Stephane Brassinnes (ONDRA/NIRAS) s.brassinnes@nirond.be	Mavrik Zavarin (LLNL) zavarin1@llnl.gov	Carlos Jove-Colon (SNL) cfjovec@sandia.gov

Brief descriptions of each work package listed in Table 3.6-1 are given below:

- WP3 – ASTRA: Alternatives RWM Strategies (0.7 M Euro, 2 years)
  - Analysis of readiness, feasibility and challenges of alternative RWM solutions needed by many countries, in particular SIMS, but also larger programs due to new requests accruing in national programs to safely manage and dispose of their waste.
- WP4 – FORSAFF: Waste Management for SMRs and Future Fuels (1 M Euro, 2 years)
  - Develop understanding and provide recommendations on SMR deployment and supplier options, with respect to nuclear waste management.

- WP8 – SAREC: Release of Spent Fuel (5 M Euro, 5 years)
  - Improved quantification and mechanistic understanding of the release of safety-relevant radionuclides covering most representative types of spent nuclear fuel (SNF) and of the fuel evolution both prior and posterior to contact with groundwater better to predict the radionuclide source term for post-closure safety assessment.
- WP9 – InCoManD: Innovative and New Container/Canister Materials (5 M Euro, 5 years)
  - Analysis of readiness, feasibility, and challenges of alternative RWM solutions needed by many countries, particularly SIMS, as well as larger programs, due to new requests accruing in national programs to safely manage and dispose of their waste.
- WP10 – ANCHORS: Hydraulic-Mechanical-Chemical Evolution of Bentonite (5 M Euro, 5 years)
  - The objective of this WP is to increase the optimization potential of bentonite barrier systems: buffer, backfill, and seals, and the Safety Case resilience 1) by qualifying the Hydro Mechanical (HM) behavior of various kind of bentonite types and mixtures through laboratory experimental program focused on heterogeneity, chemical effects and friction at different scales and 2) by improving the numerical tools that are necessary to carry out performance assessment of bentonite barriers in a Thermo-Hydro-Mechanical-Chemical (Gas) (THMC(G)) repository environment..
- WP13 – RAMPEC: Radionuclide Mobility Under Perturbed Conditions (5 M Euro, 5 years)
  - Improve the predictive capacity of models of disposal system chemistry and radionuclide mobility under perturbed conditions based on a combination of new experimental and modelling studies up to the cell scale.
- WP16 – HERMES: High-Fidelity Numerical Simulations (4 M, 4 years)
  - This WP aims to develop high-fidelity numerical models for simulations of strongly coupled THMC processes in repository nearfield, repository design optimization and interpretation of mock-up experiments using a combination of physics-based models and accelerated computing assisted with machine learning and artificial intelligence.
- WP17 – CSFD: Criticality Safety for Final Disposal (2.6 M Euro, 5 years)
  - Explore the optimization potential of the technical and administrative measures available for ensuring criticality safety in final disposal, attain an improved understanding of their methodological validation and experimental verification, and further consolidate the technical basis of the criticality safety argumentation for final disposal of fissile wastes.
- WP18 – DITUSC: Quality Assured Thermodynamics Understanding (0.5 M Euro, 2 years)
  - Thermodynamic understanding and quality-assured data support the Nuclear Waste Disposal Safety Case, with special focus on a transversal understanding.

4 BILATERAL COLLABORATION OPPORTUNITIES

International collaboration with active joint research activities can also be facilitated via direct informal or semi-formal agreements between national laboratories and international partners. Several SFWST scientists have close relationships with their international counterparts, resulting from workshops and symposia meetings, or from collaboration outside of SFWST's scope. International disposal programs benefited from collaboration with SFWST scientists and are generally quite open to including them in their ongoing research teams. This may require the preparation of a Memorandum of Understanding (MoU) 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 German Federal Ministry of Education and Research (BMWi), with the Republic of Korea, with Japan under the JNEAP (Joint U.S.–Japan Nuclear Energy Action Plan) agreement, and with France resulting from a MoU with Andra.

Sections 4.1 through 4.10 below summarize selected bilateral collaboration opportunities that emphasize access to data from international field experiments and participation of SFWST researchers in collaborative field studies. Some of the opportunities described (e.g., Germany, Republic of Korea, Sweden, Israel, France) have resulted in close collaborative research work between SFWST scientists and their international counterparts; the others describe opportunities for active research collaboration in the future. Section 4.11 discusses opportunities for international collaboration to develop best practices for site characterization and site selection via engagement with countries that currently go through such efforts at varying execution stages.

4.1 COLLABORATION OPPORTUNITIES WITH GERMANY

4.1.1 HISTORY AND STATUS OF THE GERMAN WASTE DISPOSAL PROGRAM

Germany has a long history of research and exploration work focusing on radioactive waste disposal in domal salt. However, the initially proposed and pursued Gorleben site became a highly contentious political issue in the 80s and 90s, and a moratorium on further development of the site was imposed in 2000, primarily due to political reasons. Germany's program for permanent disposal of high-level waste hit a reset button and started from scratch again. In July 2013, Germany adopted a new Act on the Search and Selection of a Site for a Repository for Highly Radioactive Waste (StandAG). As a first step, the newly created law was evaluated by a joint federal/state committee of members representing different interests, the "Commission on the Storage of High-Level Radioactive Waste." The Commission developed criteria and recommendations for selecting a repository site that ensures the best possible security for one million years. Based on the commission's final report, the further developed Site Selection Act (StandAG) was amended in May 2017. According to this Site Selection Act, all regions in Germany with suitable geologies such as rock salt, clay rock, and crystalline rock (such as granite) must be considered in a multi-stage site selection procedure, initially planned to be finalized in 2031.

Germany also redefined responsibilities for radioactive waste disposal. BGE, the Federal Company for Radioactive Waste Disposal, has been entrusted with implementing site selection procedures for a final repository, particularly for heat-generating radioactive waste. BASE, the Federal Office for the Safety of Nuclear Waste Management, is the regulator. BASE performs regulatory, licensing, and supervisory tasks concerning disposing of, storing, handling, and transporting high-level radioactive waste. The BASE also regulates the site selection procedure for a disposal site for radioactive waste, monitors the completion of the process, and organizes public participation in the search for a site. Meanwhile, BGR, the Federal Institute for Geosciences and Natural Resources (i.e., the German Geological Survey), has been tasked to provide the German Government with independent and neutral advice on all geoscientific and geotechnical issues involved in the Federal Government's nuclear repository projects.

BGE started with the search for a repository site in 2017 by identifying an initial set of areas that seemed, in principle, suitable for hosting a repository. In 2020, these areas still covered about 54% of Germany's surface area, meaning a lot of down-selection still needed to be done before a few siting regions were selected to be investigated in more detail. In August 2022, BGE announced that the reduction from a so-called "white map" of Germany to sub-areas to a few siting regions would be delayed considerably. In addition, the goal of naming a site in 2031 as stipulated by the law is expected to be missed by a wide margin. The timeline envisions a target corridor for site selection between 2046 and 2068. This speaks to the complexity of selecting a repository site starting from an entire country and comparing a broad range of host rock options, a challenge the U.S. program may also face.

With the start of the site selection procedure in 2017, Germany (like the U.S.) recognized the value and became intensely engaged in various international collaboration initiatives in geologic disposal research. For example, BGE, BASE, and BGR joined the DECOVALEX initiative and are partners in the Mont Terri Project. BGE is also a partner in the HotBENT Project and the CFM Project. BGR participates in the SKB Task Forces and the HotBENT Project. In addition, there are several research organizations with strong international connections. GRS, the Gesellschaft für Anlagen- und Reaktorsicherheit, conducts research and analysis in its fields of competence, namely reactor safety, radioactive waste management, and radiation and environmental protection (partner in the Mont Terri Project). The German Helmholtz Centers (perhaps best described as the German equivalent of DOE's national laboratories) have long-running research programs focused on safety issues relating to nuclear waste management, including the long-term safety of deep geologic repositories (participants in the DECOVALEX initiative and the Mont Terri Project). Given that the two countries are in a similar stage in terms of nuclear waste disposal, with a broad focus on a range of suitable geologies, it is no surprise that there are several ongoing collaboration projects conducted by SFWST researchers and their German counterparts, both under the umbrella of above-mentioned multi-partner initiatives or in direct bilateral collaborations. As to the latter, much of this bilateral collaboration is currently centered on salt research, as described in Section 4.2 below.

4.1.2 U.S./GERMAN SALT RESEARCH COLLABORATIONS

Over the past 15 years or so, DOE/SFWST researchers and their German colleagues in academia and other research laboratories have collaborated closely on various R&D issues related to disposal of radionuclide waste in salt, and scientists from both countries have engaged in several cooperative activities, including joint experiments, coupled-salt-mechanics modeling, and benchmarking. A MoU was signed several years ago between DOE and the German Federal Ministry of Economics and Technology (BMWi) to cooperate in geologic disposal of radioactive wastes (MoU date: November 2011). Also, fourteen 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. In FY24, the 14th U.S./German Workshop was held June 25-28, 2024, in Manchester, United Kingdom (combined with a NEA Salt Club Meeting). The overriding premise of the U.S./German collaboration is to advance the scientific basis for salt repositories.

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 4.1-1). While the moratorium on Gorleben has been lifted, R&D activities at Gorleben have not yet resumed, and it is unlikely that underground testing at this URL will ever occur again. 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 4.1-2, the TSDE experiment comprised of two parallel drifts, each of which housing three electrical heaters to simulate emplacement of heat-producing waste. SFWST scientists have used data from the TDSE experiment to validate the large-scale applicability of coupled THM models (Rutqvist et al., 2016), as part of a joint code development effort between LBNL and a research group led Technical University of Clausthal (TUC) in Germany, a world-leading research institution in salt geomechanics. Previously, the joint projects between Germany and the U.S. on salt R&D primarily focused on domal salt (e.g., Gorleben) rather than bedded salt (e.g., the Waste Isolation Pilot Plant (WIPP) facility). This changed a few years ago with the onset of the bilateral KOSINA Project and WEIMOS Projects which have now ended. Ongoing U.S./German joint projects (RANGERS, KOMPASS, MEASURES, GRS collaboration) are further described below.

Figure 4.1-1. View of one of the underground tunnels at Gorleben at the 840 m level (BMWi, 2008).

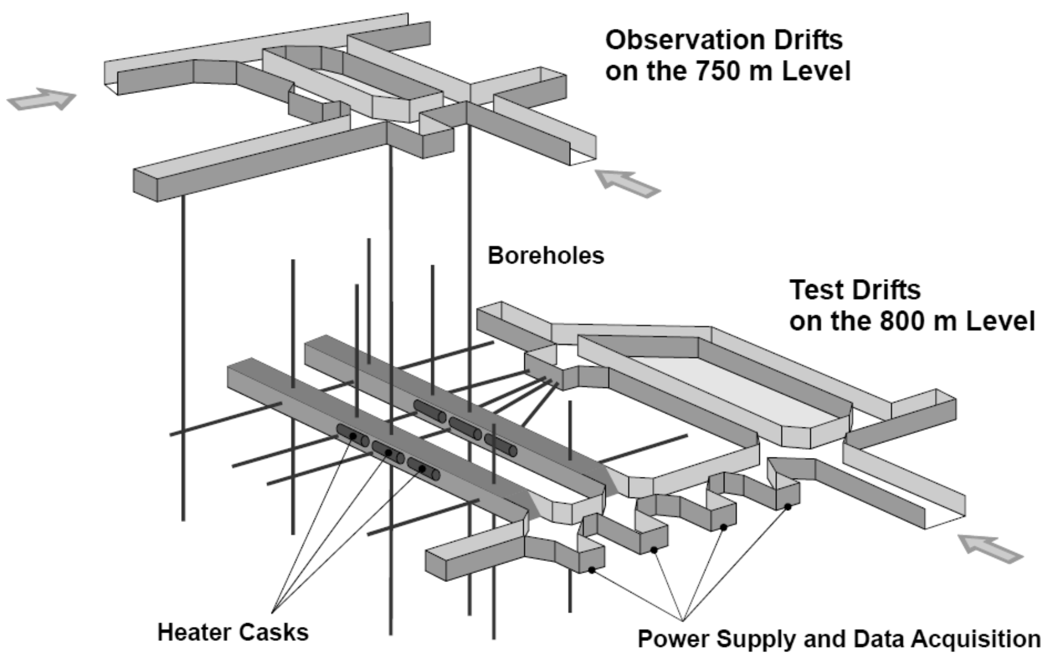


Figure 4.1-2. Schematic view of the two drift tests used in the TSDE experiment (800 m level of the Asse salt mine) (Rutqvist et al., 2015).

4.1.2.1 RANGERS PROJECT

The objective of the joint U.S.-German RANGERS project is to develop a "Design and Integrity Guideline for Engineered Barrier Systems for a HLW Repository in Salt". Despite extensive knowledge and experience about geotechnical barriers in salt formations, there is no guideline for designing and verifying such structures for a high-level radioactive waste repository. Thus, the project between SNL and BGE Technology aims at developing a guideline for the planning and the design of geotechnical barriers in salt formations. This guideline will serve as a reference manual for the conceptualization of a HLW repository in Germany or the USA. It summarizes the state of the science and art available today and gives an outlook about the technologies, which will impact the development of geotechnical barrier systems in the future. Recommendations for the design and verification of geotechnical barriers based on the state of the art in science and technology will be formulated and an overview of new concepts, building materials and technologies that will shape the state of the art of tomorrow will be given. Four sub-goals are formulated for this purpose:

- Compilation of existing knowledge and experience for the design and construction of geotechnical barriers and compilation of new concepts and technologies related to the geotechnical barriers.
- Development of a guideline based on the state of the art in science and technology for the design and verification of geotechnical barriers.
- Based on the developed guideline, preliminary design and verification of the geotechnical barrier system for selected repository systems.
- Comparison of design results according to the new guideline with results of previous design and assessment.

The RANGERS project is finishing its fifth and final year (an extension to complete reporting). Overall, the collaborative project has been a worthwhile collaboration on designing, optimizing, and modeling the engineered aspects of repositories for radioactive waste disposal in salt. Bringing together BGE TEC's expertise in mechanical modeling and SNL's expertise in flow modeling over the last five years, the RANGERS team improved its understanding of geotechnical barriers in salt formations and developed key collaborations that will continue in future collaborative efforts (e.g., EURAD-2).

See Section 6.6.2 in this report for a short summary of SFWST's FY24 RANGERS activities, and for more detailed information, see Sections 1 and 2 of the FY24 report by Mills et al. (2024).

4.1.2.2 KOMPASS AND MEASURES PROJECTS

Joint Projects KOMPASS and MEASURES are collaborations of German, Dutch, American, and British researchers seeking to improve thermo-hydro-mechanical models for crushed salt (i.e., run-of-mine or granular salt) to be used as backfill for emplacement tunnels. Partners conduct experiments to understand crushed salt behavior and further develop, calibrate, and validate models for crushed salt. The KOMPASS project included two phases (KOMPASS- 1 and KOMPASS-2), while MEASURES is a follow-up project. After translating to English, the acronym KOMPASS stands for "Compaction of Crushed Salt for Safe Enclosure," while MEASURES stands for "Multi-scale experimental and numerical analysis of crushed salt material used as engineered backfill for a nuclear waste repository in rock salt." The KOMPASS and MEASURES partners are Bundesgesellschaft für Endlagerung Technology (BGE) (Peine, Germany), Institute für Gebirgsmechanik (IfG) (Leipzig, Germany), Technical University of Clausthal (TUC) (Clausthal, Germany), Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) (Köln, Germany), Bundesanstalt für Geowissenschaften und Rohstoffe (BGR) (Hannover, Germany), Centrale Organisatie Voor Radioactief Afval (COVRA) (Nieuwdorp, The Netherlands), Utrecht University (UU) (Utrecht, The Netherlands), Sandia National Laboratories (SNL), and Nuclear Waste Services (NWS) (United Kingdom).

The first phase of the KOMPASS project was completed in 2020, with a comprehensive final report by Czaikowski et al. (2020). During this phase, experimental techniques for consolidation were thoroughly evaluated to produce adequate pre-compacted and compacted samples under various conditions, which included characterizing sufficient reference material. A total of 34 different samples were produced, and several underwent microstructural investigations to document associated deformation mechanisms. In addition to laboratory testing and analysis, model benchmarking initiatives revealed that while most models can reproduce results, they still require a well-founded laboratory database to further predict functional relationships to characterize the THM-coupled compaction behavior of crushed salt.

The second phase of the project (KOMPASS-2) was completed in 2023, with a comprehensive final report (Friedenberg et al., 2024). The focus was on investigations of microstructural effects of added moisture on pre-compaction and compaction methods. Based on results from the first phase, a systematic test series was planned to establish further reproducible and predictable correlations between stress, duration of compaction, moisture states, and respective target porosity.

During FY24, the former KOMPASS partners developed the proposal for the MEASURES project (Mills et al., 2024). This proposal retains the overall framework of the KOMPASS projects (compaction experiments, microstructural studies, and modeling), but narrows the focus to the following specific topics:

- Separating the sensitivity to mean stress, water content, and porosity
- Quantification of contributions from individual microstructural mechanisms
- Permeability measurements over a range of relevant porosities
- Calibration of constitutive models
- Quantification of uncertainties in laboratory as well as in numerical simulations

The proposal was submitted to the German Federal Ministry for the Environment, Nature Conservation, Nuclear Safety and Consumer Protection (BMUV) in late 2024 and received an “A” rating from the review committee. Once the MEASURES budget proposal is fully approved, funding would begin no earlier than Fall 2024.

See Section 6.6.2 in this report for a short summary of SFWST’s FY24 KOMPASS and MEASURES activities, and for more detailed information see Section 2 of the FY24 report by Mills et al. (2024).

4.1.2.3 COLLABORATIVE PERCOLATION EXPERIMENTS WITH GRS

In 2019, a collaborative effort began between SNL and the German GRS to perform brine and gas percolation experiments of salt cement seals in conjunction with the BATS-1 experiment and task for DECOVALEX- 2023 (Kuhlman, 2020). GRS performed similar experiments on German salt cement seals during the Full- Scale Demonstration of Plugs and Seals (DOPAS) project within the EURAD-1 program, with LAVA-2 and LASA- EDZ as sub-projects (Jantschik et al., 2018). The frame and pressure cell setup at GRS is unique and can perform THMC experiments, including brine percolation. Due to unforeseen delays from COVID-19, personnel changes at GRS, and occupied equipment for other experiments, these tests were delayed several years; however, discussions on setup and sample types continued during meetings of the US/German Workshop. The proposed tests include coupled HMC flow tests at 25°C using simulated WIPP brine, coupled THM flow tests at 60°C, and HM flow tests at elevated pressures. BATS samples have now been sent to GRS which is expected to start the experimental work in FY25 (Section 4 in Mills et al., 2024).

4.2 COLLABORATION OPPORTUNITIES WITH THE REPUBLIC OF KOREA

Several years ago, a formal commitment to collaboration on nuclear fuel management was established between the United States and the Republic of Korea (ROK). The bilateral agreement between DOE and the ROK Ministry of Science, ICT, and Future Planning (MISP) has led to a broad collaborative research program regarding utilizing civilian nuclear energy and the nuclear fuel cycle (McMahon, 2017). The two countries set up the Spent Fuel Management Working Group (SFMWG) to discuss/plan collaboration on the storage, transportation and disposal of spent nuclear fuel. Regarding active research elements centered on disposal science, bilateral R&D mainly focused on the KURT URL in Korea. KURT stands for KAERI Underground Research Tunnel, with KAERI being the Korea Atomic Energy Research Institute.

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 has a total length of 255 m with a 180 m long access tunnel and two research modules totaling 75 m. The maximum depth of the tunnel is 90 m from the peak of a mountain. The horseshoe-shaped tunnel is 6 m wide and 6 m high (Figure 4.1-1). The tunnel construction at KURT started in March 2005 and was completed in November 2006. An expansion of the tunnel completed in 2014 is shown in Figure 4.1-2, which allowed for an 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.

KURT is a relatively small and very shallow facility compared to other URLs, including those discussed in Section 3. The first 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 4.1-3). Later phases comprised additional site characterization work related to the tunnel expansion and included *in-situ* long-term performance tests on a 1/3 scale engineered barrier system at KURT. The site characterization work focused on a major water-conducting feature (MWCF), which was initially identified from surface boreholes and has since been accessed from the new expansion tunnels.

As part of their joint activities in the Spent Fuel Management Working Group, researchers at SNL and KAERI developed a multi-year plan in 2015 for joint field testing and modeling to support the study of high-level nuclear waste disposal in crystalline geologic media, which included sharing of KURT site characterization data. Two specific collaborative tasks were executed in FY16 and FY17, as follows: (1) streaming potential (SP) testing regarding correlation with groundwater flow, (2) technical data exchange regarding site characterization and buffer material specifications. Currently, there are no research activities of SFWST scientists related to KURT; however, KAERI remains open to future collaboration on various topics, including the use of KURT.

In addition to KAERI, DOE may also consider pursuing active research collaboration, including joint field experiments, with the Korean Radioactive Waste Management Agency (KORAD), the Korean implementer. A call for proposals has recently been released by KORAD together with the Republic of Korea's Ministry of Trade, Industry and Energy (MOTIE) to identify candidate sites to host a generic underground research laboratory (URL) for research into high-level radioactive waste disposal. The research facility will be used to study rock mass properties and disposal system performance about 500 meters underground. MOTIE and KORAD noted the generic URL will be built at a site entirely separate from high-level radioactive waste disposal facilities, with no radioactive waste or used nuclear fuel being taken inside the area. The underground facilities will focus on staff training and development of disposal technologies suitable for the Korean geological environment, while also providing the public with the opportunity to experience an atmosphere akin to a high-level waste disposal facility. Technologies developed in the facility will be used in the process of site selection, construction, and management of the high-level waste repository. According to current plans, the URL construction is to start in 2026 with completion scheduled for 2032. The operation period will be about 20 years, starting from 2030.

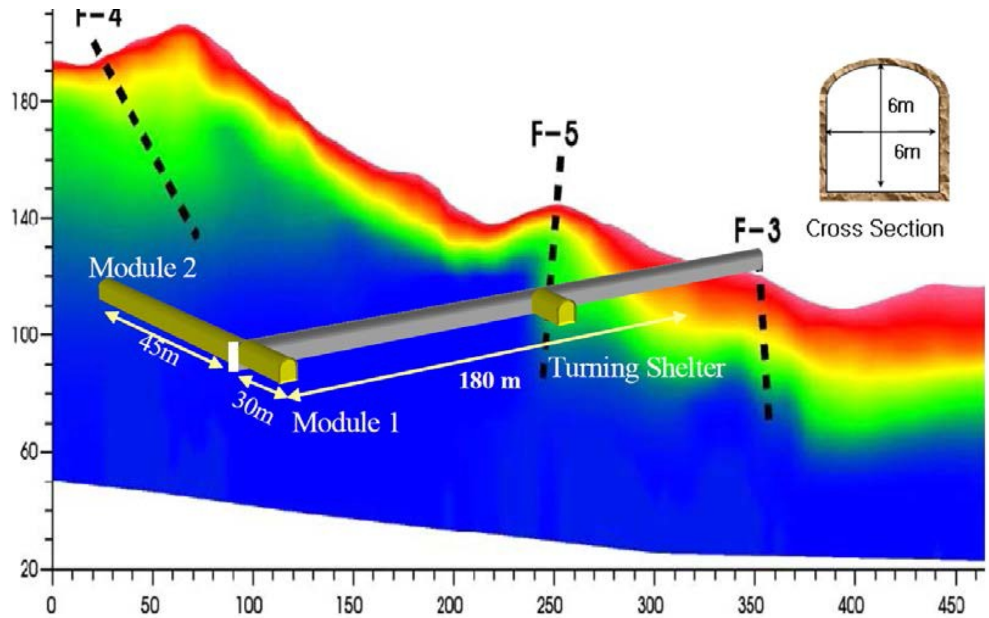


Figure 4.2-1. Layout of the KURT URL in Daejeon, Korea before extension (KAERI, 2011).

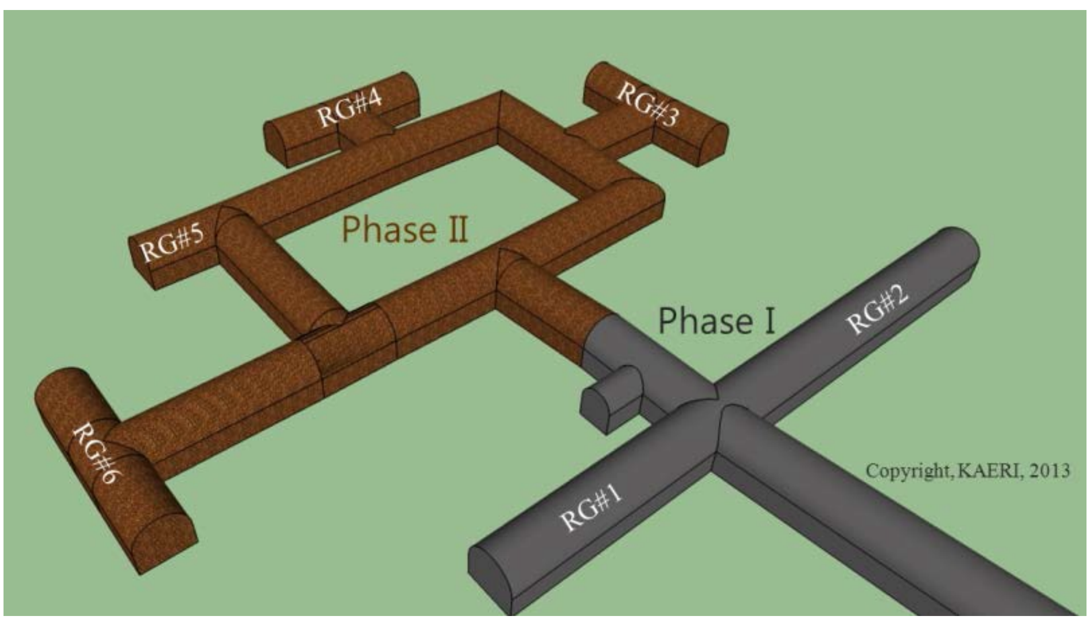


Figure 4.2-2. Layout for tunnel extension of KURT (Wang et al., 2014).

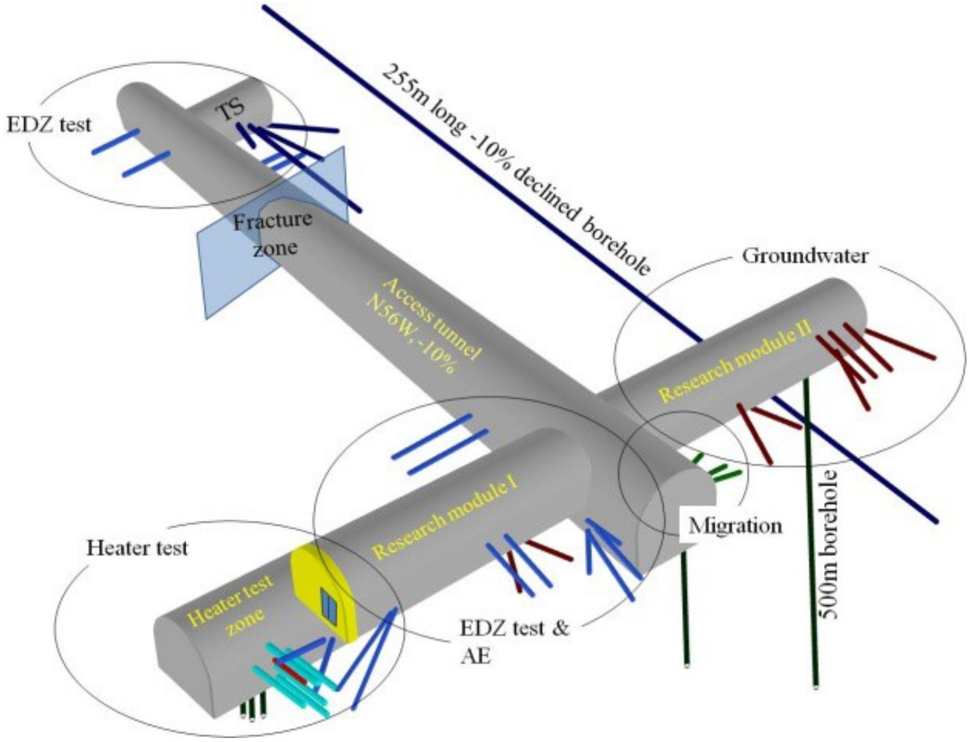


Figure 4.2-3. Location of *in-situ* tests and experiments at KURT (from Wang et al., 2014).

4.3 COLLABORATION OPPORTUNITIES WITH COSC, SWEDEN

In addition to collaboration with Sweden under the umbrella of the SKB task forces (Section 3.4), DOE researchers have participated in the "Collisional Orogeny in the Scandinavian Caledonides" (COSC) project, a scientific deep drilling project in Sweden. COSC's objective was to gain insights into the tectonic evolution of the area, characterize present and past deep fluid circulation patterns, determine current heat flow to constrain climate modeling, and characterize the deep biosphere. Another objective of this project was to calibrate high quality surface geophysics through deep drilling. In 2014, a deep borehole (COSC-1) was drilled into the crystalline basement to a depth of 2,495.8 m with a core recovery of greater than 99%. The borehole was drilled though the Seve Nappe formation, which contains high-grade metamorphic rocks indicative of deep (100 km) crustal levels (Figure 4.3-1). The main lithologies encountered consist of felsic, amphibolite, and calc-silicate gneisses, amphibolite, migmatites, garnet mica schist, with discrete zones of mylonite and microkarst. In addition to drilling the well and collecting core, the research team also conducted pre-drilling and post- drilling seismic and other geophysical surveys, borehole geophysical logs, conducted on-site measurement on recovered cores, carried out systematic X-ray fluorescence (XRF) measurement on all cores at 10 cm intervals for key chemical compositions, and performed downhole spectral gamma ray (SGR) logging to determine U, Th and K contents all along the borehole.

SFWST recognized that the COSC project provided a valuable opportunity to test characterization techniques for crystalline host rocks. In FY15, LBNL initiated a joint R&D program on fluid-logging testing using the first COSC borehole. The joint research's main objective was to understand better what information can be obtained from core and borehole measurements and how best to characterize the deep subsurface environment in granitic and other crystalline rocks in the context of nuclear waste disposal. LBNL gained key insights on the use of the flowing fluid electrical conductivity (FFEC) logging tool to identify deep flowing fracture zone in crystalline basement.

In FY16 and FY17, LBNL conducted laboratory measurements of transmissivity of fractured core samples from the COSC-1 well as a function of controlled stress. These fractured core samples were spatially correlated with fluid flow zones in the same well identified by flowing fluid electrical conductivity (FFEC) logs, thereby confirming the field measurements. In FY18 through FY20, LBNL researchers further examined the hydraulic properties of crystalline rock cores from the COSC-1 well using a unique laboratory-scale apparatus that allowed for measuring the multi-directional transmissivity to assess fracture anisotropy under confining stress conditions. Experimental results for two cores, 211-2 and 401-1 (from the 702 m and 1241 m depths, correspondingly), were examined in detail, including developing a preliminary numerical model of the fracture planes and conducting numerical simulations of the laboratory flow experiments. In FY24, LBNL reexamined the details of the experimental design and realized that the aperture distribution to model a specific flow experiment did not incorporate an extremely high aperture section caused by a chunk of rock breaking off from the surface. A new model was created using the correct aperture distribution and the results were reexamined, particularly the relative transmissivity values across the core in four directions.

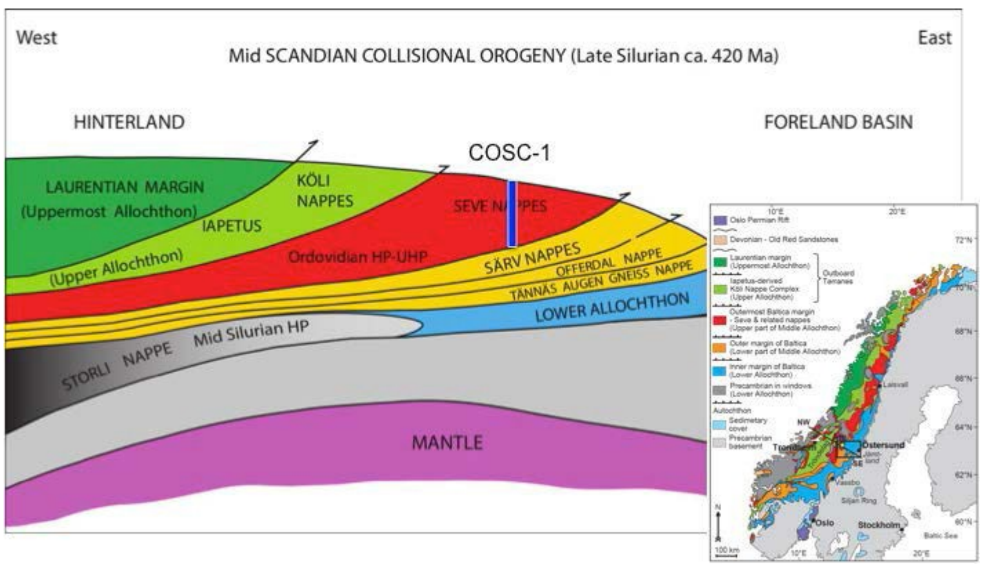


Figure 4.3-1. Location of COSC-1 deep borehole (Dobson et al., 2016).

In the summer of 2019, LBNL together with its Swedish partners conducted a new field-testing campaign in the COSC-1 well to probe the coupled HM and chemical processes in selected fracture zones, comparing transmissive and not transmissive fractures (Guglielmi et al., 2019, 2020). This work was done using an innovative downhole fracture characterization device, the SIMFIP tool, which can be used to measure real-time 3D mechanical deformation of a borehole interval, containing one or more fractures, together with measurements of the injection water flow rate, pressure, temperature, and water electric resistivity. The following field tests were carried out: pressure buildup tests, pressure falloff tests, and constant flow rate tests for each of the three intervals.

In FY21, after the field tests were finalized, LBNL started with a comprehensive analysis and interpretation of the field-testing results. In FY22, LBNL scientists explored how the observed *in-situ* fracture responses could best translate into generic fracture network models (including their hydrogeologic properties) of the host rock close and away from repository tunnels. A new approach was developed for *in-situ* estimation of fractured rock elastic properties from SIMFIP measurements and for linking these elastic properties with the development of stress heterogeneity within a fractured hard rock. In FY23 and FY24, LBNL scientists continued their analysis of measurements of water flow, pressure, and displacements from the COSC-1 borehole to develop a multi-step monitoring workflow for the *in-situ* characterization of fractures including their hydromechanical properties and stress states. This workflow was independently demonstrated in FY24 to characterize a fault zone at 1 km depth in the Bedretto URL in Switzerland (see Section 4.5). See Section 6.8.2 in this report for a short summary, and for more detailed information see Section 3 of Hu et al. (2024).

4.4 COLLABORATION OPPORTUNITIES WITH THE BEDRETTO URL, SWITZERLAND

In addition to Mont Terri (Section 3.1) and the Grimsel Test Site (Section 3.3), Switzerland has another deep URL The Bedretto Lab, situated in the Swiss Alps and accessed from a 5 km long tunnel with an average overburden of ~1 km of crystalline rock, provides a unique testbed for deep geosciences experiments and has straightforward access to a natural inactive Alpine fault zone (Figure 4.4-1).

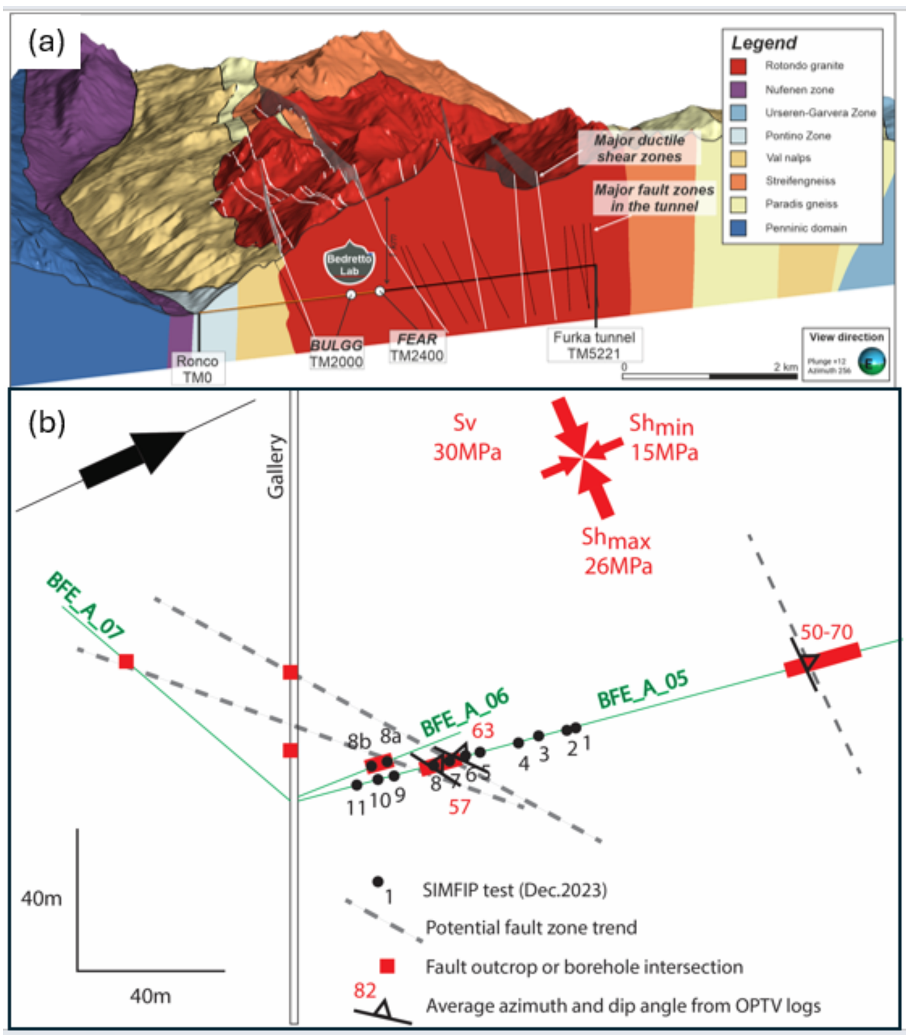


Figure 4.4-1. (a) Bedretto underground laboratory with the FEAR tests set in the Rotondo granite in Switzerland. (b) A detailed map shows the boreholes (green lines) drilled across the fault zone. Black dots with numbers 1 to 11 show the SIMFIP tests conducted in borehole BFS-A-05 to estimate stress variations across the fault zone (grey dashed lines) and fault properties (Hu et al., 2024).

In preparation for a fault activation experiment (FEAR project in collaboration with ETHZ), a borehole has been drilled through the fault zone for fault HM properties characterization and stress estimations. The fault extends > 200 m in either direction from the Bedretto tunnel, and it is reasonably well-oriented for slip to occur in the present-day regional stress field. Preparation of the FEAR experiment provided a unique opportunity to apply the COSC-developed workflow for fracture/fault characterization (Section 4.3). Compared to the COSC-1 borehole, the demonstration at Bedretto could test (1) whether an inactive fault zone can induce significant variations in the stress tensor's orientation and magnitudes, and (2) whether HM fault zone properties at 1 km depth are much different from shallower settings.

Field testing of the workflow using the SIMFIP probe in Bedretto was conducted between November 30 and December 9, 2022. Eleven tests in pre-defined sections were successfully carried out. Three tests above and seven below the fault zone in intact and partially fractured rock were conducted, and a cross-hole test in the fault zone at 38 m depth in BFE_A_05. Analysis of the experiments in FY24 was promising, showing that the workflow could be successfully applied to detect stress tensor rotation caused by an inactive fault zone in a very deep crystalline setting. This confirms the maturity of the SIMFIP deep borehole screening procedure for crystalline fractured rock. See Section 6.8.2 in this report for a short summary, and for more detailed information see Section 3 of the FY24 report by Hu et al. (2024).

4.5 COLLABORATION OPPORTUNITIES WITH ISRAEL

The Israel Atomic Energy Commission is examining the possibility of locating a geological waste disposal site within the carbonate Ghareb and Nezer Formations in the northern Negev, Israel (Klein-BenDavid et al., 2019). A research program is underway in Israel which includes studies to better quantify and predict chemical interactions along interfaces between cementitious materials and the carbonate host rocks. Such interactions may lead to chemical and structural alteration of both the cement and the host rock caused by diffusion and reaction driven by gradients in porewater pH and composition, pore structure, and mineralogical differences between the different materials. In FY22, researchers from the Nuclear Research Center of the Negev in Israel and of SNL conducted a joint study to simulate the long-term performance of interfaces between cementitious materials (CEM I, selected as a bounding case for alkali cement-rock interactions, and a low pH cement) with carbonate geologic strata (limestone, chalk, marl, oil shale, low organic phosphorite and high organic phospharite). This study has now ended. For the U.S. program, this collaboration provided insights into the specific challenges of using carbonate rocks as host rocks for permanent disposal or interim storage. Also, the methods for long-term predictions of interfacial reactions between cement and carbonate are relevant for other interfacial materials as well.

4.6 COLLABORATION OPPORTUNITIES AT ANDRA'S LSMHM URL, FRANCE

The major underground disposal research facility in France is Andra's LSMHM (Laboratoire de recherche Souterrain de Meuse/Haute-Marne) 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 the Bure URL 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 4.6-1, 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 4.6-2). DOE and Andra have a Memorandum of Understanding (MoU) which covers any bilateral research collaboration on clay/shale disposal and use of the LSMHM. This would be in addition to the collaborative work of U.S. and French scientists under the umbrella of the DECOVALEX initiative. As mentioned earlier, Andra managed Task A of the most recent DECOVALEX-2023 phase, with focus on field experiments on thermal and gas fracturing at the Bure URL (Section 3.2.2.1), and is currently leading Task BaSSIS on gas migration in sand-bentonite sealing systems in DECOVALEX-2027 (Section 3.2.3.5).

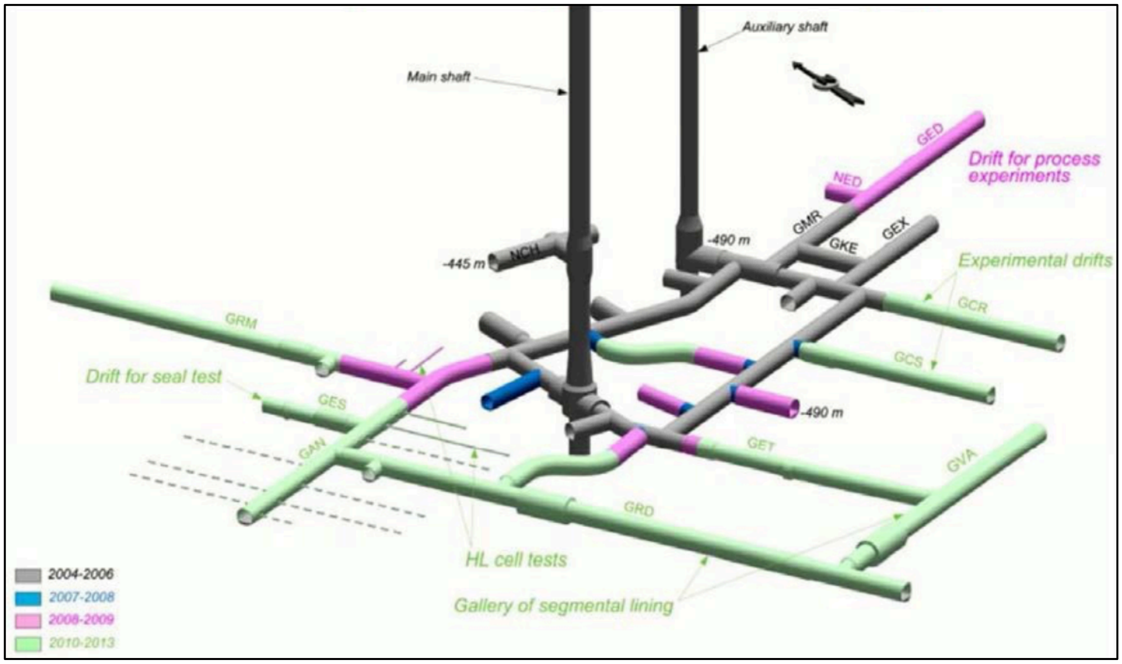
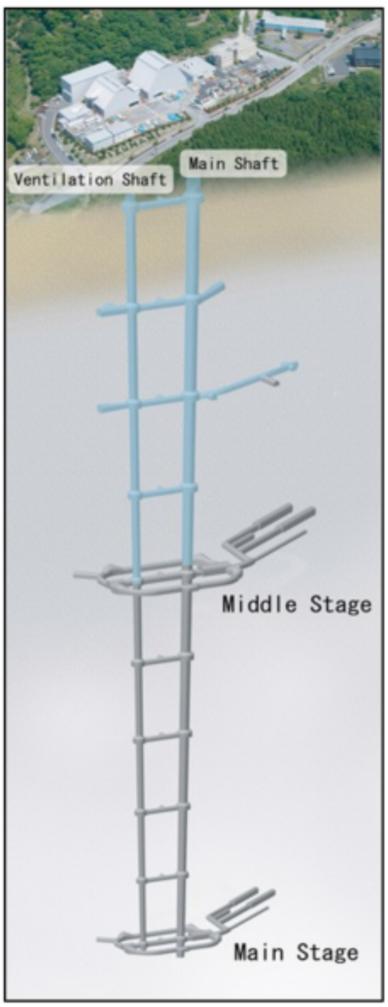


Figure 4.6-1. Layout of the LSMHM URL at Bure, France (Lebon, 2011).

Figure 4.6-2. LSMHM URL at Bure, France (from http://www.andra.fr/download/andra-international- en/document/355VA-B.pdf).

4.7 COLLABORATION OPPORTUNITIES AT JAEA'S URLS IN JAPAN

Opportunities for active collaborative R&D in underground research laboratories in Japan exist at the Horonobe URL in sedimentary rock and at the Mizunami URL in crystalline rock (Figure 4.7-1). 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 have also been a frequent partner in many of the cooperative initiatives that DOE has joined in recent years (Section 3, Table 3.1-1), and both nations collaborated for several decades under the umbrella of the DECOVALEX initiative. In the most recent completed DECOVALEX phase, JAEA coordinated a modeling task related to EBS behavior at the Horonobe URL based on a full-scale *in-situ* experiment (Section 3.2.2.4). A new opportunity for collaboration with JAEA has recently emerged with the launch of the Horonobe International Project (HIP), a partnership of currently eight international organizations, collaborating under the umbrella of the NEA, to demonstrate advanced technologies in the design, operation and closure of a repository in a sedimentary (mudstone) formation (Section 3.5.7).



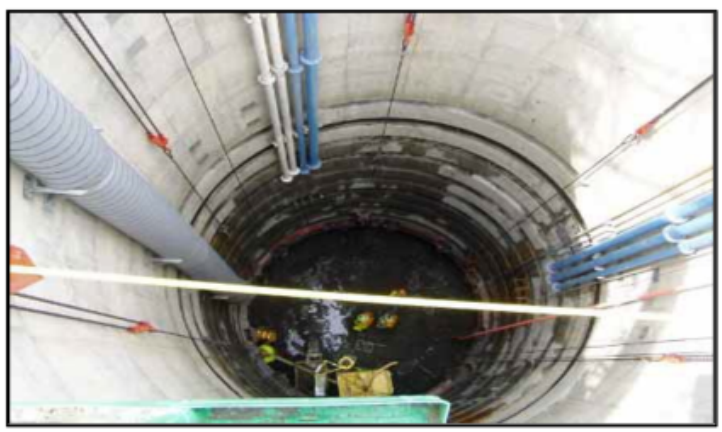


Figure 4.7-1. Layout of the Mizunami Underground Research Laboratory in Japan (left), and photo of tunnel shaft construction (right).

4.8 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 4.8-1). 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, which is discussed in more detail below. The Belgium organizations involved in conducting and interpreting these experiments have long-standing relationships with DOE/SFWST scientists; they are open to participation with SFWST 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, mainly because the geologic conditions in the HADES URL are not relevant to the premier host rock options in the U.S.

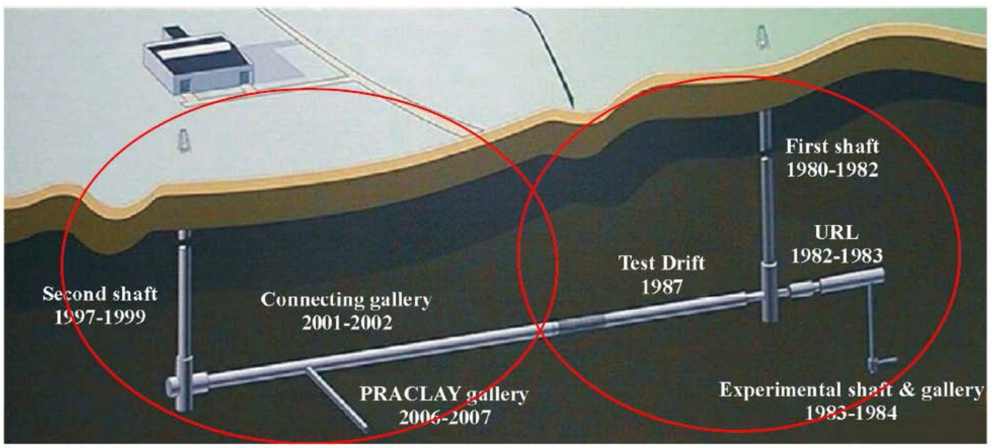


Figure 4.8-1. Layout of the HADES URL in Mol, Belgium (Li, 2011).

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 involves a 30 m gallery section to be heated for about 10 years with many monitoring sensors (Figures 4.8-2), for the purpose of investigating the 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. The heating phase of the test started in January 2015. Once the heating phase is over (probably in late 2024 or 2025) and the entire experiment has been dismantled, scientists will spend time analyzing all the data and drafting their final conclusions. The results of the PRACLAY experiment will refine existing knowledge about the behavior of the Boom Clay when subjected to heat. The main objective is to confirm that heating does not impair the clay's ability to physically contain the radioactive waste. It is therefore a crucial step in the process of developing and implementing a repository in soft clay.

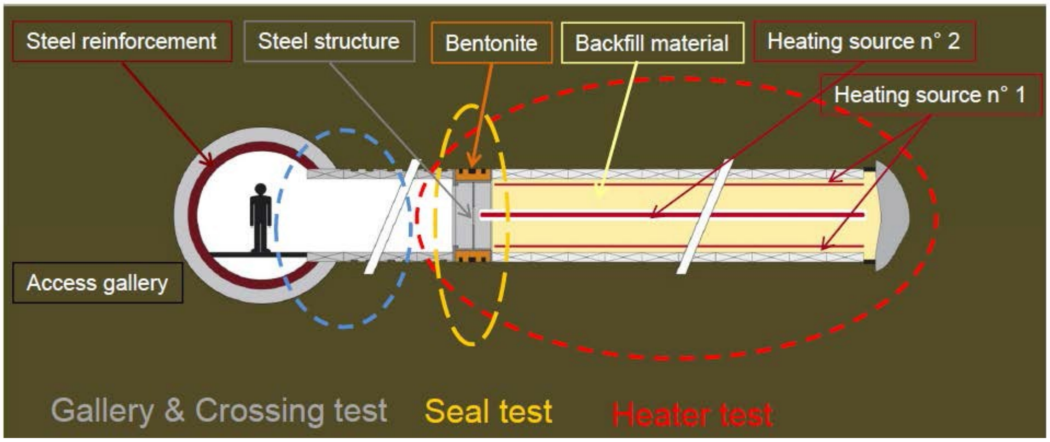


Figure 4.8-2. Layout of the PRACLAY *in-situ* experiment at HADES URL (Li, 2011).

4.9 COLLABORATION OPPORTUNITIES AT ONKALO URL AND DISPOSAL SITE, FINLAND

The status of the Finnish program is very advanced compared to other nations: The program has already selected a site, has submitted a license to operate, and has started construction of its final disposal facility Onkalo near Olkiluoto. In the initial phase, Onkalo was primarily an underground research facility, where studies were carried out to confirm the suitability of Olkiluoto bedrock for final disposal. In 2015, after years of research in the URL, Posiva received the disposal facility construction license from the Finnish Government and the repository is now being constructed to a depth of 400–450 m. Onkalo consists of a spiral-shaped access tunnel, vertical shafts, tunnels, and technical rooms. The access tunnel takes the form of a downward spiral and reaches the technical facilities level at about 437 m. Emplacement will occur in some 50 km of tunnels be excavated in bedrock. Figure 4.9-1 shows rendering of the layout of Onkalo while it was primarily being used as a research facility, showing the access tunnels and shafts, deposition tunnels, as well as research and demonstration areas. Details may be found in POSIVA OY (2011) and Aalto et al. (2009).

At the time of writing this report, Posiva is about to embark on a final step of getting ready for waste emplacement at Onkalo, the so-called Trial Run of Final Disposal. The Trial Run is the final phase of Posiva's preparing for the operation of the repository. It will be carried out with the methods, procedures, equipment and personnel to be used in the operation phase. Posiva has invited international programs to participate as observers in the Trial Run and learn how the entire disposal process functions. Discussion with Posiva's experts will help gain insights to benefit other national programs (Jalonen, 2024).

In terms of research collaboration, researchers from the U.S. and Finland have in past years participated in the modeling interpretation of the REPRO diffusion experiment at Onkalo, which was a modeling task conducted under the umbrella of the SKB GWFTS Task Force (see Section 3.4.2.1). These activities have ended and there are no current bilateral research activities between the two programs related to the Onkalo URL. However, as pointed out in Section 3.2.3.6, the recent construction activities provide a wealth of relevant new data from pilot hole and deposition tunnel investigations, such as fracture frequencies, fracture trace maps, and groundwater inflows. These new data are now being used in the FRESCIP task of DECOVALEX-2027, proposed by the Swedish regulator SSM. The task will jointly evaluate previous and new fracture data to understand whether the PA modeling may be impacted by the additional learnings from dense tunnel data.

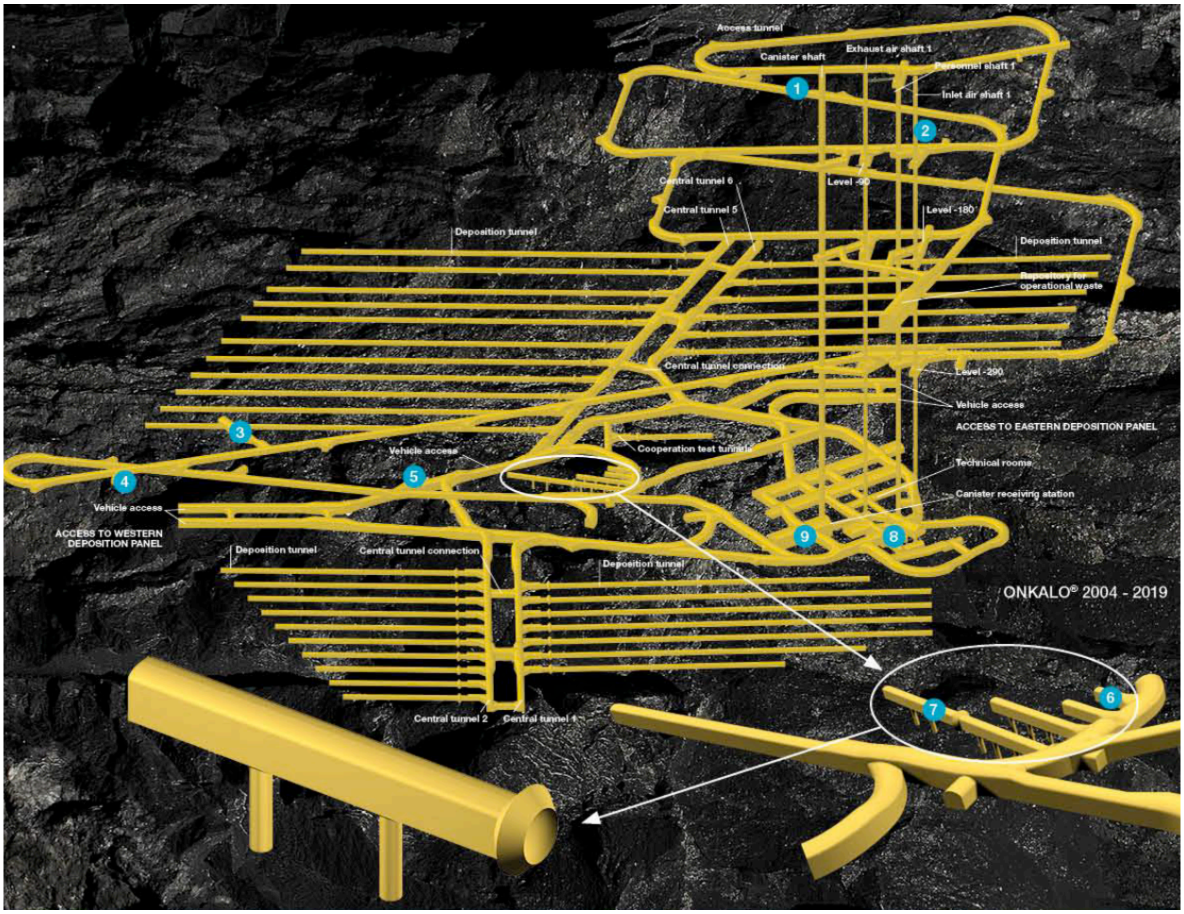


Figure 4.9-1. Layout of the Onkalo URL in Finland. Numbered areas 1-5 are research niches, 6-9 are demonstration tests and other tests. Source: Jalonen (2024).

4.10 COLLABORATION OPPORTUNITIES AT BUKOV UNDERGROUND RESEARCH FACILITY, CZECH REPUBLIC

SÚRAO, the radioactive waste management authority of the Czech Republic, has an ambitious geologic disposal program focusing on the nation's granitic host rock environments. Czech researchers working on disposal issues are well connected international; SÚRAO has been a member of DECOVALEX for several years and is also a partner in the HotBENT Project and the SKB's task forces.

About a decade ago, SÚRAO identified the Bukov Underground Research Facility (URF), located at a depth of 550 meters below the surface, as an ideal site for the research and evaluation of the geological environment as part of the deep geological repository development program (Dohnálková, 2024). As with similar facilities of its type, it makes use of a pre-existing underground mine infrastructure, namely the former Rožná I uranium mine. The laboratory is situated in highly metamorphosed rocks - migmatites, amphibolite, paragneiss. The underground areas of the URF are close to the B-1 and B2 shafts and are made up of a system of crosscuts, drifts, and experimental galleries and test chambers (Figure 4.10-1). Construction for the first stage – Bukov URF I - started in 2013 and was finished in 2017 (Figure 4.10-2). The facility was excavated using various technological methods and mine working dimensions in such a way that the testing of different solutions in different geological environments helped to determine the final design. Following a site characterization phase, SÚRAO embarked on a comprehensive experimental phase at Bukov and actively reached out to the international community for partnerships as the experimental research program was executed. Current research is performed in seven designated scientific areas, with 2023 experimental activities listed in Table 4.10-1.

- VEP1 – Geological Characterization Meetings
- VEP2 – Monitoring
- VEP3 – Transport
- VEP4 – Engineered Barrier Systems and THMC processes
- VEP5 – EDZ Evaluation
- VEP6 – Technological Procedures
- VEP7 – Demonstration Experiments

As research in Bukov URF I is ongoing, SÚRAO is already expanding its experimental area for new experiments with the buildout of a second stage, referred to as Bukov URF II. The experiments are designed to test the long-term interactions of materials and the effects of the environment of these materials. A priority topic is the verification of heat distribution from the waste packages through the bentonite material into the host rock (Dohnálková, 2024).

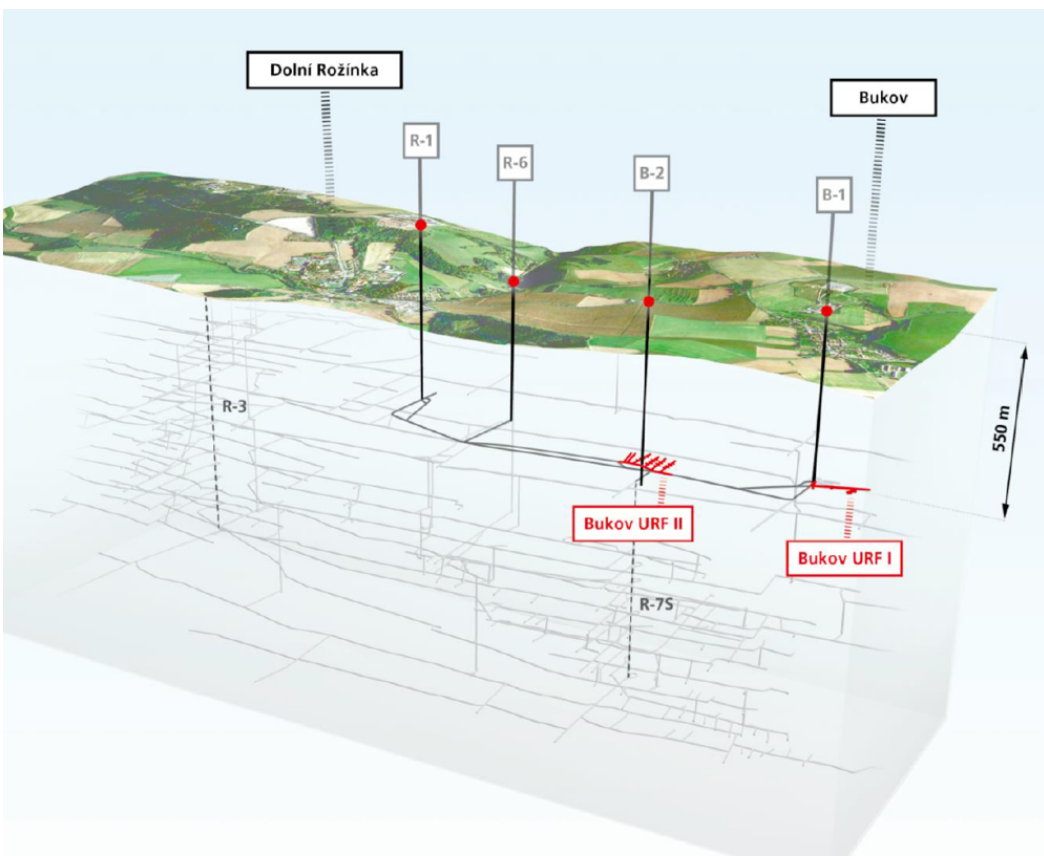


Figure 4.10-1. Schematic layout of the research areas in the Bukov URF (from Dohnálková, 2024).

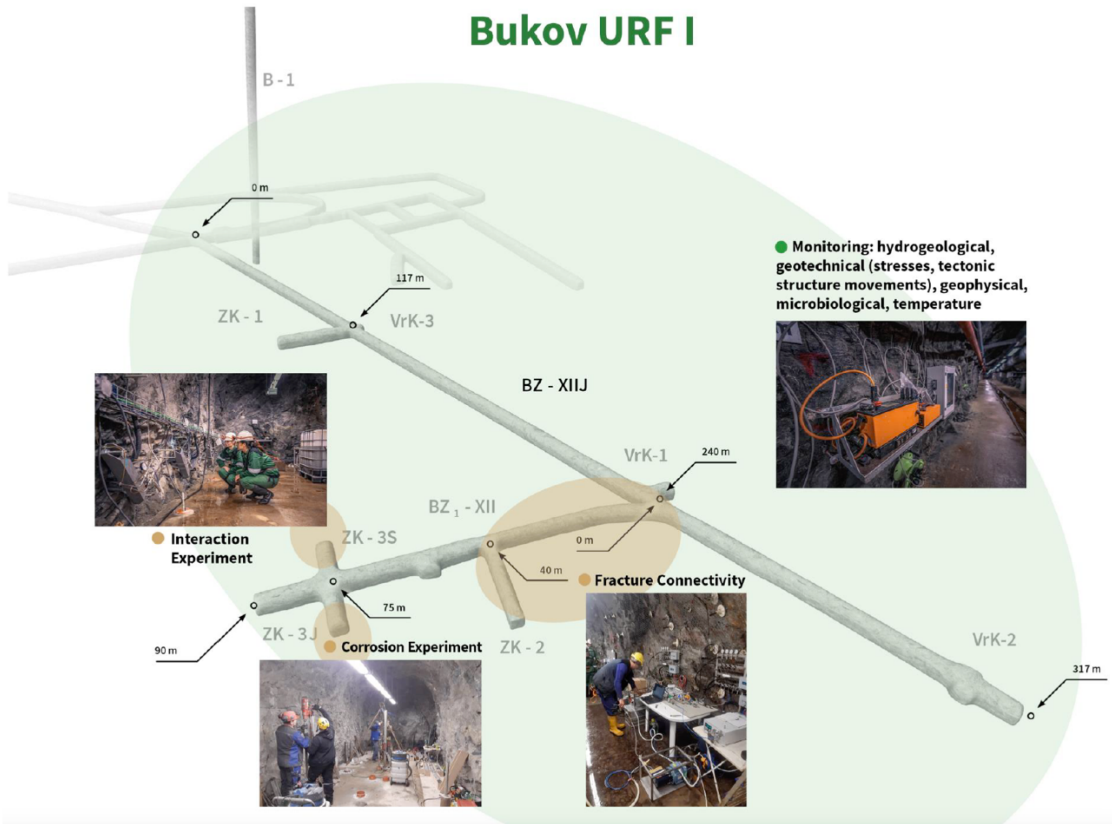


Figure 4.10-2. Major experiments conducted in the Bukov URF I area (from Dohnálková, 2024).

Table 4.10-1. 2023 portfolio of experimental activities in Bukov URF (from Dohnálková, 2024).

Name of the area	Programme area SÚRAO
Rock classification systems	VEP1
Characterisation of EDZ and EIZ	VEP5
Advection-dispersion transport processes	VEP3
Diffusion processes	VEP3
Model concepts in groundwater flow	VEP3
Uncertainties in in-situ transport parameters	VEP3
Flow in EDZ and EIZ	VEP5
Testing the implementation and characterisation of disposal bore holes	VEP6
Concrete with lowered pH	VEP4
Long-term laboratory	VEP4
Experimental study of THM(C) processes - HEAT experiment	VEP4
Bentonite erosion and colloid transport (ERO)	VEP4
Buffer expansion to backfilled and WDP load (EXP)	VEP4
Prototype repository demonstration experiment (DEMO)	VEP7

4.11 COLLABORATION OPPORTUNITIES AT BEISHAN URL IN CHINA

As a major nuclear nation with a long-standing geological disposal program, China has embarked on an ambitious plan to develop area-specific underground research laboratories in representative rock formations (Wang, 2014). China is moving swiftly with URL site selection and characterization plans; the current idea is that the country would focus on a granite site first, followed by a clay formation. The granite formations in the Beishan area, located in northwestern China's Gansu Province, have been selected as the most suitable area for a high-level waste repository in China. This is based on an abundance of favorable host rock geologies, with eight large granite intrusions identified as suitable subareas. The Beishan area has other advantages as well: the region has favorable socio-economical and natural conditions, characterized by highly sparse population, no useful farmland, lack of mineral resources, and generally poor economic potential. At the same time, Beishan can be easily reached with convenient transportation options. In terms of potential clay sites, China focuses on two regions of possible interest. These are the Tamusu and the Suhongtu regions within the Bayingebi Basin, located in the Inner Mongolia region. The Beijing Research Institute of Uranium Geology (BRIUG) manages China's geological disposal program, which is open to international cooperation. In fact, with the IAEA coordinating, BRIUG over the past decade has closely worked with several countries, including the U.S., for technical guidance and practical advice related to their URL program, for example, related early siting criteria, site selection approaches, and specific site characterization techniques.

In 2021, China started construction of its first underground research laboratory in the Beishan area. According to the current design, the URL will have a sizeable expandable research space at two main working levels (280 m and 540 m below the surface), accessed by a ramp and a personnel shaft (Figure 4.11-1). Construction has progressed as planned: As of May 2024, the shaft has been completed, the ramp has been advanced to a length of 4,000 m using a tunnel boring machine, and excavation of the first working level has started (Wang and Liu, 2024). Research to be conducted includes site characterization activities (some of which have already begun as the excavation occurs, such as geological and hydrogeological mapping), testing of engineering technologies and engineered barriers, and safety assessment activities such as monitoring of radionuclide release and migration behavior. It is expected that underground *in-situ* testing will take place until 2050. The final stage – the construction of the disposal facility – is planned to take place from 2041 to 2050, assuming the *in-situ* testing confirms the area's suitability (Carter and Nieder-Westermann, 2021).

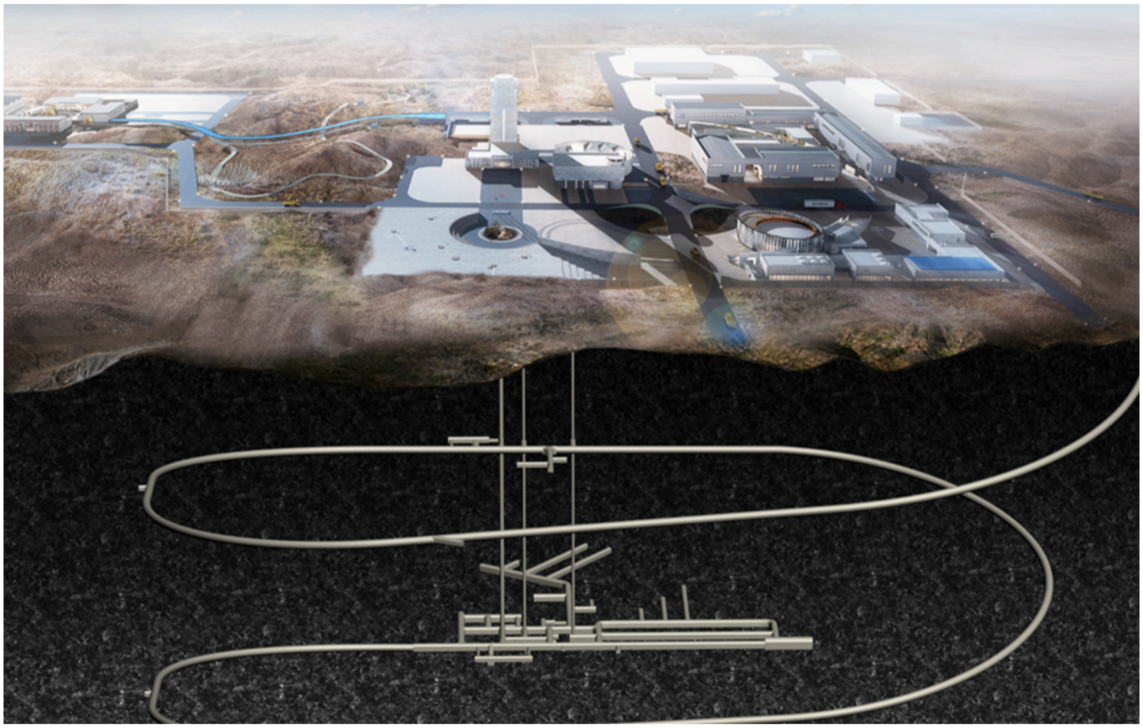


Figure 4.11-1. Design of the planned URL in Beishan, China (Carter and Nieder-Westermann, 2021).

4.12 COLLABORATION OPPORTUNITIES TO DEVELOP BEST PRACTICES FOR SITE SELECTION AND CHARACTERIZATION

As the SFWST campaign continues to evolve and may at some point transition from generic R&D to disposal implementation, an important goal for international collaboration will be to gain knowledge about international siting approaches and site characterization practices, via engagement with countries that currently go through such efforts. Countries that come to mind are, for example, Germany which is currently in the early stages of site selection considering the entire country and a broad range of host rocks, Canada which has narrowed its search from initially 22 volunteer areas to two sites, and Switzerland which has just down selected from three siting regions to one. Such international collaboration would involve close observation and information exchanges, to review the spectrum of participatory siting approaches considering different end member cases (e.g., begin with volunteer communities vs. begin with entire country and down-select based on geologic considerations), and thereby gain a better understanding of best practices and lessons learned. For example, DOE managers, engineers and scientists may be sent abroad to work in such a spectrum of siting programs for an extended time (say 6 months or a year). In addition, the campaign could review site characterization strategies, methods, and plans from advanced programs, especially Canada and Switzerland because they are conducting site characterization now. Furthermore, SFWST scientists could be actively collaborating with or embedded in ongoing international site characterization efforts, for example, via joint development and *in-situ* application of surface- and borehole-based characterization tools. Below is a summary of the program status in Germany, Canada, and Switzerland:

- Germany: The German implementer BGE started with the search for a repository site in 2017, by identifying an initial set of areas across the <u>*entire country*</u> that seemed in principle suitable for hosting a repository. In 2020, these “suitable areas” still covered about 54% of Germany’s surface area, meaning a lot of down-selection still needed to be done before a few siting regions were selected to be investigated in more detail. In August 2022, BGE announced that the reduction from a so-called “white map” of Germany to sub-areas to a few siting regions would be delayed considerably. In addition, the goal of naming a site in 2031 as stipulated by the law is expected to be missed by a wide margin. The current timeline envisions a target corridor for site selection between 2046 and 2068. This speaks to the complexity of selecting a repository site starting from an entire country and comparing a broad range of host rock options, a challenge that the U.S. program may also be facing.

- Canada: The process to select a repository site for Canada’s spent nuclear fuel started in 2010, when the country began asking for *volunteer sites* to come forward. The Canadian implementer, NUMO, made it clear from the beginning that the program would only move forward at a site with informed and willing hosts. By 2012, twenty-two communities voluntarily expressed interest in learning more about the project and exploring the potential to host it. Currently, after a gradual process of narrowing down through increasingly intensive social engagement and technical site evaluation via a comprehensive drilling program, two areas remain as potential hosts, both in Ontario: the Wabigoon Lake Ojibway Nation (WLON)-Ignace area with a granitic host rock and the Saugeen Ojibway (SON)-South Bruce area with a low-permeability sedimentary host rock. A decision for one of these two sites to move forward into the regulatory decision-making process is expected for late 2024 or early 2025 (Swami, 2024).
- Switzerland: Site selection of deep geologic repositories in Switzerland is governed by the Sectoral Plan, which defines three siting stages. Stage 1 started in 2008 with a *down-selection from the entire country* of Switzerland per pre-defined exclusion criteria. (This stage is identical to the current status in Germany.) At the end of Stage 1, the Swiss implementor Nagra defined six regions for further consideration in Stage 2, which by the end of that second stage in 2018 had been reduced to three regions. These three regions, named Jura Ost, Nördlich Lägern and Zürich Nordost, are in the northern part of the country /near each other. All regions feature the same host rock, the Opalinus Clay, with only moderate variations in characteristics and properties. Based on a detailed characterization and drilling program, Nagra was able to demonstrate in 2024 that the post-closure safety of deep geological repositories can be ensured in all three siting regions. Furthermore, Nagra concluded that Nördlich Lägern is the safest siting region of the three, as it offers the best geological barrier, a higher stability against erosion, and a high degree of flexibility for the layout of the repository (Müller-Germanà, 2024). Nagra is soon to submit the license application for the Nördlich Lägern site, which is then to be reviewed by the regulator ENSI till 2030.

5 SELECTION AND RE-EVALUATION OF INTERNATIONAL COLLABORATION TASKS

5.1 COLLABORATION PLANNING AND RE-EVALUATION

Starting in 2012 with an emphasis on international collaboration, DOE became a formal partner in several multinational initiatives that promote active joint research, often with specific focus on URL field experiments and related data: the Mont Terri Project (since 2012), the DECOVALEX initiative (since 2012), the CFM Project (2012 - 2015), the FEBEX-DP Project (2015 - 2018), the SKB Task Forces (since 2014) and the HotBENT Project (since 2018) (Sections 3.1 - 3.4). As a result, SFWST researchers have been in a position for more than a decade now that allows for participation in planning, conducting, and interpreting the many past and ongoing field experiments associated with these initiatives, and they do so in close collaborative partnerships with international scientists. DOE also reached out to—and explored options of collaboration with—individual international disposal and other research programs, such as from the Germany, Republic of Korea, Sweden, Switzerland, Israel, France, Japan, Belgium, Czech Republic, Finland and China (Section 4), which have led to several bilateral joint R&D activities.

In FY12, when SFWST decided to focus on active international collaboration as a strategic emphasis for DOE's disposal research, the campaign first developed a set of guiding principles for the selection of collaboration options and activities, as follows:

1. Focus on activities that complement ongoing disposal R&D within SFWST (e.g., the science and engineering tools developed in SFWST are tested in comparison with international experiments) and that align with goals, priorities, and funded plans of the SFWST program.
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 (i.e., U.S. researchers work closely together with international scientists on specific R&D projects relevant to both sides).

Starting from these principles, the campaign initiated a planning exercise to identify the most relevant and promising international opportunities and to select and develop a set of activities that align with the goals, priorities, and funding plans of the SFWST. In a general sense, the benefits of international collaboration are obvious: SFWST can gain substantial value from the knowledge, data, and modeling capabilities that international partners have developed over decades of research. In terms of specific activities, 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. The SFWST campaign had identified such open R&D issues in several planning exercises, as summarized for example in Wang (2010) and Jové-Colón et al. (2010), and in a roadmap exercise prioritized them by importance to the safety case (Nutt, 2011, Tables 7 and 8).

As part of the initial planning exercise, SFWST management and scientists developed a comprehensive table of international opportunities to provide a basis for the selection of international activities. The table listed the most relevant ongoing or planned field experiments conducted in international URLs, provided information on how SFWST participation can be achieved, which research areas would be the main benefactor (generally either EBS or NBS), 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. Detailed planning of an initial set of international activities was then conducted in three workshops held in FY11 and FY12. The objectives of these workshops were: (1) to inform DOE leadership and SFWST scientists about existing or future international opportunities, and (2) to align SFWST work package activities with opportunities for international collaboration. The first workshop was a session held in conjunction with the SFWST Working Group Meeting in Las Vegas in July 2011, at this point mostly for informative purposes. The second workshop, held in Las Vegas in April 2012, was a full-day meeting to review the current and planned work scope within SFWST 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 SFWST program. A third workshop was held in conjunction with the SFWST Working Group Meeting in Las Vegas in May 2012, to inform SFWST researchers about the outcome of the full-day planning workshop, to present them with the collaboration options, and to initiate active R&D participation.

As research priorities changed over the years and new opportunities for collaboration have emerged, SFWST's international research portfolio evolved, and it will continue to evolve in the future. Therefore, the campaign has made a targeted effort to re-evaluate its international collaboration activities, in a process similar to the initial planning phase in 2012. Planning sessions were held in conjunction with the annual SFWST Working Group Meetings to review existing and emerging opportunities for international collaboration, evaluate their technical merit and cost/benefit ratio, to align these opportunities with the current and planned work scope within SFWST 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 SFWST program. For example, as a result of this process, SFWST decided in FY15 to end its participation in the CFM Project because of its relatively narrow focus and relatively high participatory cost.

In FY18 and FY19, the SFWST campaign initiated a detailed re-planning effort to ensure that all disposal research activities were aligned with and of high relevance to the safety case. Starting at the SFWST Working Group Meetings in Las Vegas in May, 2018 and continued/finalized at a dedicated R&D Roadmap Update Workshop in Las Vegas in January 2019, all ongoing and planned research activities were discussed in the context of their priority score, which in turn was evaluated by answering two important questions: (1) how important is the knowledge gained from a given research activity in terms of the three safety case elements (pre-closure safety analysis, post-closure safety assessment, confidence enhancement) and its technical basis, and (2) what is the state of the art level that the research activity would support (in other words, a given research activity would be most important when it addresses fundamental gaps in methods or data). The former was measured with the so-called ISC score (Importance to Safety Case), ranging from low importance (ISC = 1) to high importance (ISC = 5). The latter was evaluated using the so-called SAL score (State of the Art Level), ranging from well understood (SAL = 1) to fundamental knowledge gaps (SAL = 5). Priorities were then assigned by a score matrix that combined both scores, with the highest priorities assigned to research activities that were both important to the safety case and still had fundamental knowledge gaps. Detailed results from this roadmap update are given in the report by Sevougian at el. (2019), which summarizes the progress of ongoing disposal R&D activities since 2012, re-evaluates R&D priorities for all existing activities, and identifies new activities of high priority.

International collaboration activities, and their integration with other generic research tasks, were included in this broad activity-based priority assessment conducted in 2018. In addition to reviewing the benefits of ongoing activities, the participating experts evaluated several new international collaboration opportunities, e.g., the new tasks proposed for the upcoming DECOVALEX-2023 phase, and some planned Mont Terri, GTS, or SKB experiments. Priority scoring considered emerging R&D needs recognized by the international community (e.g., the issue of gas pressure buildup in response to gas generation from corrosion) or emerging priorities in the SFWST campaign, such as R&D on disposal of DPCs which now contain a significant fraction of the Nation's commercial spent fuel activity. The resulting expert scores for international activities were categorized into "high-priority," "high- to medium priority," and "medium priority" (Sevougian et al., 2019). The highest-scoring items included research activities on high-temperature impacts in bentonite and clay, gas generation and transport, fault slip and development of flow paths, and coupled processes in salt. None of the international activities, current or planned, scored lower than "medium."

In FY20, the DOE requested development of a formal plan for activities in the SFWST disposal research portfolio over 5 years. SFWST campaign leadership then worked across several control accounts to discuss the 5-year direction of the campaign. It developed a report that serves as a strategic guide to the work within the disposal research R&D technical areas (i.e., the control accounts), focusing on the highest priority technical thrusts (Sassani et al., 2020). The 5-year plan, as well as its FY21 and FY23 updates (Sassani et al., 2021; 2023), distinguishes the near-term (i.e., the more certain 1- to 2-year timeframe) and the longer term (less specific 3- to 5-year) timeframe. The near-term emphasis can represent the present R&D portfolio with modest modifications that reflect emerging priorities and funding levels. In contrast, the 3- to 5-year period represents a longer-term vision of where the SFWST disposal research portfolio is heading provided there is no major external change to the program direction. According to this plan, international collaboration will remain an important cross-cutting campaign activity over the next five years, with regards to opportunities involving *in-situ* experiments in underground research laboratories across a range of geologic systems.

Below is a synopsis of the 1- to 2-year and 3- to 5-year planning elements defined for international collaborations in disposal research (Sassani et al., 2023), moderately updated for this FY24 report.

Near-Term Topics (Next 1- to 2-year period)

- *Continue participation within international R&D in underground research laboratories for a range of geologic systems*

  As mentioned above, the current international research portfolio, which spans across several technical areas including Argillite Disposal R&D, Crystalline Disposal R&D, Salt Disposal R&D, EBS R&D, and GDSA, has been re-evaluated and re-prioritized in 2019 as part of a broad activity-based priority assessment across the campaign (Sevougian at el., 2019). As such, the 5-year plan suggests that these priorities will remain largely intact over the next few years, while moderate revisions to the international portfolio will be made as new opportunities emerge and existing collaborations end. Note that some key international activities involve long-term *in-situ* experiments that will continue for years to come (e.g., the full-scale FE Heater Test at Mont Terri, HotBENT), while others such as DECOVALEX tasks have a limited timeline and will occasionally be replaced with new collaborative tasks.

- *Continue assessment of new international opportunities*

  Ongoing evaluation of existing and emerging opportunities for international collaboration is a key responsibility of the International Collaborations technical area. We will continue to review, assess, and develop such opportunities in close integration with international partners, will evaluate technical merit and alignment with the current and planned work scope within SFWST work packages, and revise the portfolio of international R&D activities as appropriate. Examples of recent collaboration activities that SFWST has recently considered and evaluated include:

  - The new DECOVALEX-2027 phase, which started in the Spring of 2024, comprises eight tasks of high relevance to SFWST (Section 3.2.3). SFWST worked with DECOVALEX leadership to shape the task portfolio and ultimately decided to participate in this new phase.
  - SFWST considers tunnel, shaft and borehole sealing elements as a priority theme for engineered barriers research. Participation in relevant international experiments was recently evaluated (e.g., the SW-A Sandwich Experiment at Mont Terri, which tests a promising layered technology for shaft seals, see Sections 3.1.5.1 and 3.2.3.4; or Andra's

NSC experiment at Bure which examines a gas permeable seal, see Section 3.2.3.5). It was ultimately decided to join collaborative modeling of the SW-A Sandwich Experiment under the umbrella of the DECOVALEX-2027 initiative.

  – SFWST recently evaluated and later instituted a technical partnership with the EURAD-2 European Commission collaborative research program which initiated a new round of repository R&D work for a 5-year period from 2024 through 2029 (see Section 3.6). The goal is to encourage in-kind collaboration of SFWST scientists with projects funded under EURAD-2, for cross-benefit between these two large programs.
  – SKB has started dismantling of the inner Section of their Prototype Repository Heater Test at the Äspö HRL, Sweden (Section 3.4.4). The full-scale test started in 2001 and is now the longest operation of a multi-barrier repository experiment in the world. SKB has invited the international community to participate in the dismantling project. Scientists from SFWST met a few times with SKB in early 2023 to get clarity about the benefits and costs of joining the project as a research collaborator. Both SFWST and SKB have expressed their mutual interest and SKB recently prepared a draft contract for DOE to consider. Currently, DOE is reviewing the draft contract.

- *Pursue a more active role in conducting experimental work in international underground research laboratories)*

  The SFWST campaign will continue evaluating 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 conducting its own experimental program in international URLs. The advantage of active planning is that the experimental focus and design can be better tailored to the campaign's needs. In recent years, SFWST has already shifted towards a more active approach in shaping the future R&D portfolio of international initiatives. More such active collaborations will be considered in the future.

- *Contribute to integration and confidence building for Generic Disposal System Analysis (GDSA)*

  The international research activities, focusing on modeling and comparative analysis for complex *in-situ* experiments, ultimately lead to better predictive models and thus directly contribute to confidence building for post-closure PA models. In the SFWST campaign, the work packages for international collaboration, for generic research on EBS and host-rock specific topics, and for GDSA need to be well integrated to make optimal use of improved process models leading to better safety assessments models. The international technical area can contribute to this goal. Confidence in PA models can also be enhanced by comparing PA methods to international standards, or by benchmarking PA studies against international data sets. Under leadership of SFWST scientists, the performance assessment task in the most recent DECOVALEX phase compared PA methodologies for generic salt and generic crystalline repositories across multiple international disposal programs (Section 3.2.2.6). Comparative modeling is continued in the current DECOVALEX-2027 phase (Section 3.2.3.8), pushing further into UQ/SA.

Longer-Term Topics (Next 3- to 5-year period)

International collaboration will continue to be a central element of SFWST Campaign's disposal R&D over the next 5 years and beyond. And as research priorities change and new opportunities for collaboration present themselves, the international research portfolio will be re-prioritized as appropriate. Many of the 2-year themes discussed above will continue to drive the campaign planning. In addition, depending on the direction of the campaign and the progress made, international collaboration could be expanded to in several ways to serve other objectives. Here are two examples:

- *Develop best practices and technologies for site selection and characterization*

  The current campaign focus in disposal research is to: (1) provide a sound technical basis for multiple viable disposal options in the U.S., (2) to assess the suitability and geographic distribution of host rock types, (3) to increase confidence in the robustness of generic disposal concepts, and (4) to develop the science and engineering tools needed to support disposal concept implementation. As the campaign evolves, a suitable goal for international collaboration may be to support site characterization for site screening and site selection via engagement with countries that currently go through such efforts at varying execution stages. Such collaboration would involve close observation and information exchanges to review the spectrum of participatory siting approaches considering different end member cases (e.g., begin with volunteer communities vs. begin with the entire country and down-select based on geologic and other considerations) and thereby gain a better understanding of best practices and lessons learned. For example, DOE managers, engineers, and scientists may be sent abroad to work in such a spectrum of siting programs for an extended time (say 6 months or a year). In addition, the campaign could review site characterization strategies, methods, and plans from advanced programs, especially Canada and Switzerland, because they are conducting site characterization now. Furthermore, SFWST scientists could be actively collaborating with or embedded in ongoing international site characterization efforts, for example, via joint development and *in-situ* application of surface- and borehole-based characterization tools. SFWST's international collaborations with the Swedish COSC program and the Bedretto URL are examples of joint research efforts on site characterization methods that benefit both partners (Section 6.8).

- *Utilize international activities for training/education of junior staff*

  International collaboration has provided valuable datasets from underground testing that are not only relevant to the SFWST's campaign R&D objectives but also provided for complex scientific challenges of high interest to young researchers. The campaign will continue to make a dedicated effort to use international collaboration activities as an opportunity to recruit and train early-career scientists to become the next-generation workforce for disposal research in the United States. An essential step in this direction is the three-year workforce development pilot program launched in FY22 at LBNL, SNL, and LANL. The program aims to attract, train and advance a talented and diverse future workforce by providing interesting learning/research challenges and attractive work-abroad opportunities in conjunction with SFWST's multiple international collaboration partners (Section 6.10).

One of the near-term topics in the 5-year plan in Sassani et al. (2023) calls for DOE to move from the primarily participatory role in ongoing *in-situ* experiments conducted by other nations to an active role in developing and conducting international experiments. While there are no immediate plans for DOE to conduct its experiments in international URLs of opportunity, SFWST's disposal program has already started taking a much more active approach in shaping the future R&D portfolio of the international initiatives it has joined as a partner. For example, with Jens Birkholzer of LBNL serving as the Chair of the DECOVALEX Project, SFWST scientists have been very influential in the project's task selection and are now leading two of the current DECOVALEX-2027 modeling tasks, one focusing on the BATS heater test at WIPP and one comparing different performance assessment approaches (see Sections 3.2.3.3 and 3.2.3.8, respectively). SFWST researchers are also leading a new modeling task in the SKB EBS Task Force, which at its center has a high-temperature column experiment conducted at LBNL (Section 3.4.3.3). In addition, DOE has co-developed the planning and design of the HotBENT Project with international partners, and the full-scale high-temperature heater experiment was conducted at the GTS (Section 3.3.2). SFWST is considering establishing a Center for International Collaboration in Disposal Research to elevate international collaboration in disposal research to a new level of emphasis and recognition.

5.2 OVERVIEW OF THE INTERNATIONAL COLLABORATION PORTFOLIO

Today, more than 10 years after its initiation, the international disposal program within SFWST 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:

- **Engineered Barrier Integrity**: What is the long-term stability and retention capability of backfills and seals? 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? Is gas pressure increase and gas migration a concern for barrier integrity?
- **Near-Field Perturbation**: How important are thermal, mechanical, and other perturbations to a host rock (such as clay and salt), and how effective is healing or sealing of the damage zone in the long term? How reliable are predictive models for the strongly coupled THMC (thermal-hydrological-mechanical-chemical) behavior of clay and salt formations?
- **Flow and Radionuclide Transport**: How does high temperature affect the diffusion and sorption characteristics of clays (i.e., considering the heat load from dual-purpose canisters)? What is the potential for enhanced transport with colloids? Can transport in diffusion-dominated (clays, bentonites) and advection-dominated systems (fractured granites) be predicted confidently?
- **Integrated System Behavior, Performance Assessment, and Site Characterization**: Can the early-time behavior of an entire repository system, including all engineered and natural barriers and their interaction, be measured and demonstrated? Can this integrated behavior be reliably predicted? Are the planned construction and emplacement methods feasible? Which characterization and monitoring methods are suitable for site selection and performance confirmation? How reliable are performance assessment models?

Figure 5.2-1 gives a visual overview of the major international experiments conducted in various countries that SFWST researchers have participated in since 2012, either as active members of the experimental team or as researchers involved in the interpretative evaluation and model interpretation of the experimental data (see list of experiments in Table 5.2-1). Experiments in bold denote currently active collaborations. The figure tries to graphically illustrate the balance and focus of SFWST's international program over the past years. There are a few notable observations:

- Going from the center outward, one can see that SFWST's research is well balanced between EBS focus, near-field focus and far-field emphasis.
- Several experiments address at the same time EBS behavior and near-field processes, which comes as no surprise because *in-situ* experiments in URL tunnels by design have near-field host rock impact even if the main emphasis may be on the engineered barrier behavior.
- There are many activities related to field experiments argillite and crystalline host rock, whereas less international work has been conducted for salt. This can be explained by the U.S. program having its own salt URL in the bedded salts at the WIPP in New Mexico, so there is less need for international research outside of the U.S.
- The topic of "Integrated System Behavior, Performance Assessment, and Site Characterization" features two full-scale demonstration experiments with SFWST participation, the FE Heater Test at the Mont Terri URL in Switzerland and the EBS Experiment at the Horonobe URL in Japan. In addition, SFWST is currently considering participation in the dismantling of SKB's Prototype Repository Heater Test, another demonstration experiment that has been running since 2001 at the Äspö Hard Rock Laboratory. SFWST also participates in the field-testing of new site characterization methods and workflows, such as at the COSC deep drilling site in Sweden, the

FEAR testing at the Bedretto URL in Switzerland, and the analysis of fracturing data from the Onkalo URL and repository site in Finland.

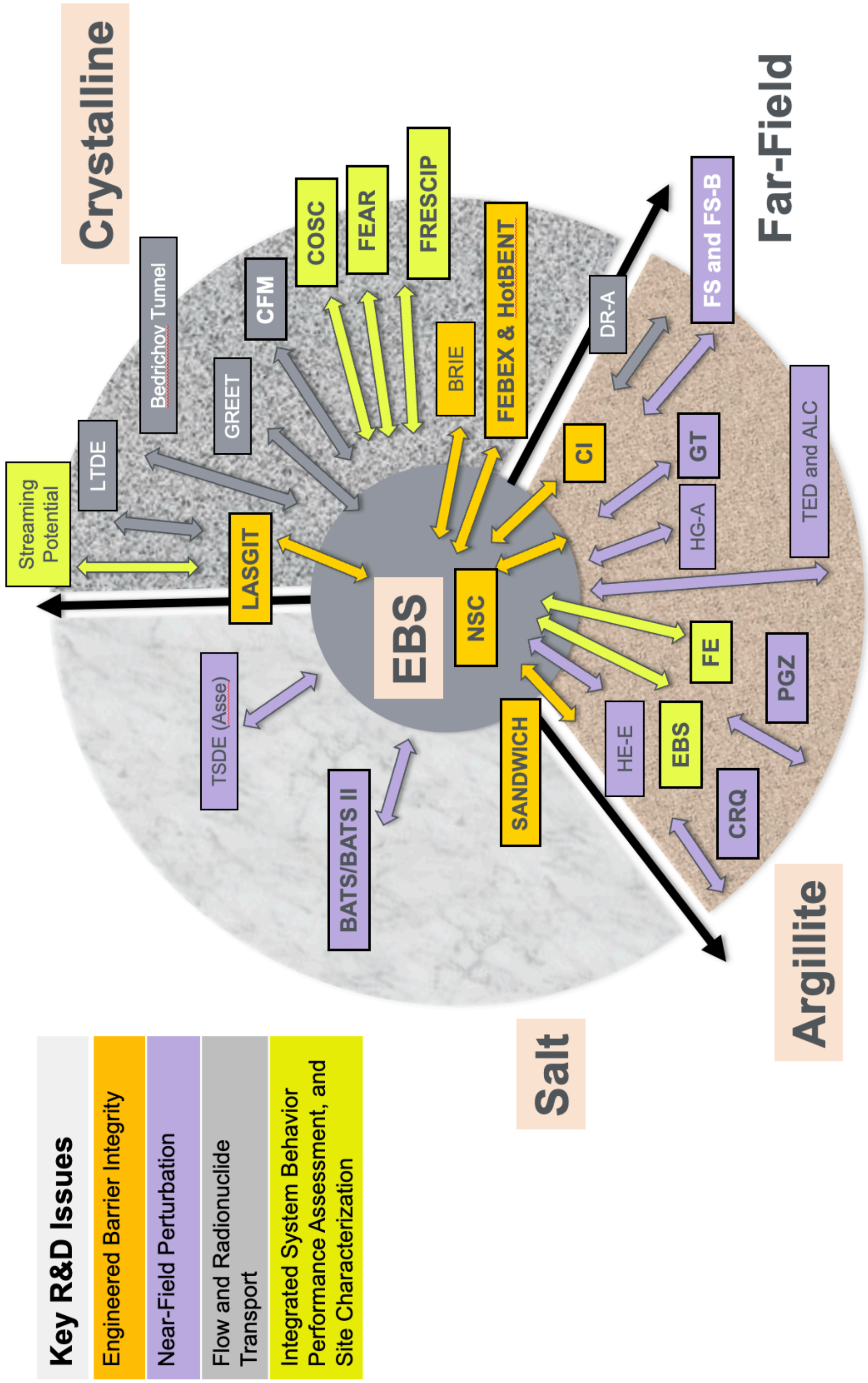


Figure 5.2-1. A high-level overview of the major international URL experiments conducted in various countries that SFWST researchers have participated in since 2012. Experiments in bold denote currently active collaborations. See Table 5.2-1 for more information on each experiment. Status: FY24.

Table 5.2-1. A high-level overview of the major international URL experiments conducted in various countries that SFWST researchers have participated in since 2012. Experiments in bold denote currently active collaborations. Status: FY24.

Key Topics	International Experiment	URL	Main R&D Focus
Engineered Barrier Integrity	Bentonite-Rock Interaction Experiment (BRIE)	Äspö HRL, Sweden	Understand the impact of flowing fractures in crystalline rock on bentonite saturation, integrity and erosion
	Full-Scale Engineered Barrier Experiment - Dismantling Project (FEBEX-DP)	Grimsel Test Site, Switzerland	Dismantling and sampling of long-term test evaluating the long-term integrity and performance of heated bentonite
	Large-scale Gas Injection Test (LASGIT)	**Äspö HRL, Sweden**	***In situ* monitoring of gas migration processes in bentonite buffer**
	HotBENT Experiment	**Grimsel Test Site, Switzerland**	**Complex THMC behavior of EBS materials up to 200 degrees C at the canister/bentonite interface**
	SANDWICH Experiment	**Mont Terri, Switzerland**	**Testing the HM behavior of a novel shaft-sealing system with alternating sealing layers**
	NSC Bentonite-Sand Sealing Experiment	**Bure, France**	**Evaluating the seal performance of a gas permeable bentonite-sand mixture at full tunnel scale**
Near-Field Perturbation	Heater Experiment E (HE-E)	Mont Terri, Switzerland	Bentonite/rock interaction to evaluate sealing and clay barrier performance at elevated temperature
	Thermal Experiment (TED) Full-scale Emplacement Test (ALC)	Bure, France	Upscaling THM simulations from lab tests to repository scale
	Gas Path Though Host Rock Experiment (HG-A)	Mont Terri, Switzerland	Evaluation of flow paths through the near-field damage zone and specifically along seals
	Thermal Simulation for Drift Emplacement (TSDE)	Asse Mine, Germany	Model benchmarking studies for thermal-hydrological-mechanical behavior salt heater test
	CRQ Thermal Fracturing Experiment	**Bure, France**	**Testing the behavior of argillite host rock to a thermal fracturing stress regime**
	PGZ Gas Fracturing Test	**Bure, France**	**Testing the behavior of argillite host rock upon high-pressure gas injection**
	Fault Slip Experiments FS and FS-B	**Mont Terri Switzerland**	**Fault reactivation and permeability generation due to repository-induced effects in a clay rock**
	Brine Availability Test in Salt (BATS)	**WIPP, USA**	**Monitoring brine distribution, inflow, and chemistry from heated salt using geophysical methods and direct liquid & gas sampling**
	GT Experiment	**Mont Terri, Switzerland**	**HM testing of argillaceous host rock responding to gas injection and migration**
	STIMTEC Experiment	**Reiche Zeche, Germany**	**Fluid injection into crystalline rock mass and measurements of microseismicity**
Flow and Radionuclide Transport	Bedrichov Tunnel Experiment	Bedrichov, Czech Republic	Interpretation of water inflow patterns and tracer transport behavior in fractured granite
	GREET (Groundwater Recovery Experiment)	Mizunami, Japan	Evaluation of early resaturation behavior in crystalline rock looking at flow behavior and chemical-biological interactions upon resaturation
	Long-Term Sorption Diffusion Experiment (LTDE)	Äspö HRL, Sweden	Monitoring the diffusion behavior in fractured crystalline rock
	DR-A Experiment (Diffusion Retention and Perturbation Test)	Mont Terri, Switzerland	Ion diffusion through compacted clay where electro-chemical charges affect transport behavior
	Colloid-Facilitated Radionuclide Migration Test (CFM)	**Grimsel Test Site, Switzerland**	**RN transport of bentonite colloids compared in a shear zone in fractured granite**
Integrated System Behavior, Performance Assessment, and Site Characterization	Streaming Potential Test	KURT, Korea	Testing a new site characterization technique to measure deep groundwater flow
	Engineered Barrier System (EBS) Experiment	**Horonobe, Japan**	**Full-scale studies of the thermo-hydro-mechanical-chemical (THMC) behavior of the EBS**
	Full-scale Emplacement Experiment (FE)	**Mont Terri, Switzerland**	**Full-scale demonstration experiment, one of the largest and longest-duration heater tests**
	COSC Experiment	**Deep Drilling Project, Sweden**	**Testing new methods and workflows for borehole-based HM fracture characterization**
	FEAR Experiment	**Bedretto, Switzerland**	**Fault characterization and reactivation in deep crystalline rock**
	FRESCIP	**Onkalo URL, Finland**	**Fractured rock characterization and inflow prediction using data from repository construction**

6 GEOLOGIC DISPOSAL RESEARCH ACTIVITIES ASSOCIATED WITH INTERNATIONAL COLLABORATIONS

Section 6 summarizes ongoing international R&D activities conducted by SFWSTD scientists collaborating with researchers from other countries. These activities involve the participation of U.S. researchers in experiments conducted in URLs, analysis of laboratory experiments, benchmarking modeling studies, development of thermodynamic databases, advances in site characterization and monitoring methods, comparisons of PA models, and a pilot program to develop a next-generation workforce in geologic disposal science. The high-level summaries of current R&D activities are prepared based on the FY24 milestone reports provided by SFWST researchers from LANL, LBNL, LLNL, and SNL (see a list of FY24 milestone reports in Section 8 “References”). The structure of Section 6 is as follows:

- Section 6.1 summarizes experimental and modeling investigations focused on understanding coupled THMC processes in the EBS. Research activities are associated with three full-scale EBS heater experiments: two are the FEBEX-DP experiment and the HotBENT experiment hosted at the Grimsel Test Site (GTS) in Switzerland, and the third is the EBS Experiment hosted at the Horonobe URL in Japan.
- Section 6.2 describes SFWST’s various international research activities that evaluate and model interactions between engineered barrier systems and host rocks based on laboratory and field experiments and reactive transport modeling.
- Section 6.3 focuses on the THM modeling of heater experiments conducted in argillaceous rock, the full-scale Mont Terri FE Experiment in Switzerland and the CRQ Thermal Fracturing Experiment at the Bure URL in France. Both activities are modeling tasks associated with the DECOVALEX-2023 initiative.
- Section 6.4 provides results of modeling of gas migration in compacted clay-based sealing materials, such as clay rock or bentonite, to understand the fate of repository gases generated over long periods from canister corrosion or radioactive decay of the waste. This research is conducted under the umbrella of the international DECOVALEX initiative and comprises the modeling of a full-scale field experiment LASGIT.
- Section 6.5 summarizes two international collaboration activities on modeling coupled processes, fluid flow, and transport in fractured crystalline rock. A micro-scale hydromechanical modeling activity related to the DECOVALEX-2023 initiative is complemented by larger-scale fracture network modeling to improve our understanding of multi-scale flow channelization in fractured crystalline rock conducted under the umbrella of the SKB Task Forces.
- Section 6.6 focuses on international collaboration activities related to coupled processes and brine migration in salt as a host rock, including investigations of the behavior of engineered barriers in salt repositories (RANGERS project), the development of improved THM models for crushed salt (KOMPASS and MEASURES projects), and the international modeling of the BATS heater test at WIPP as part of DECOVALEX-2023 Task E and DECOVALEX-2027 Task C, which are conducted under the SFWST leadership.
- Section 6.7 summarizes ongoing international studies on the possibility of the reactivation faults and fractures caused by repository-induced effects. These activities revolve around controlled injection fault reactivation experiments conducted at the Mont Terri URL.
- Section 6.8 summarizes the development and testing of advanced characterization and monitoring techniques in cooperation with the COSC deep drilling project in Sweden and the Bedretto URL in Switzerland. These international field- and modeling-based collaboration

activities are undertaken to improve understanding of flow and transport processes in fractures in crystalline rocks under fluid pressure or stress variations, such as the effects of deformation, shear displacement, dilation, and propagation.

- Section 6.9 describes collaborative activities to improve post-closure performance assessment and radionuclide transport predictions based on (1) collaborative modeling of crystalline and salt reference cases under the umbrella of the DECOVALEX-2023 initiative and (2) the development of thermodynamic databases and thermochemical databases as part of the international NEA Thermochemical Database (TBD) Project.
- Section 6.10 summarizes a pilot program launched at LBNL, SNL, and LANL to develop a next-generation workforce in geologic disposal science. The program uses international collaboration activities to attract, train and advance junior staff.

Table 6-1 provides a roadmap through Section 6 and its sub-sections, including references to the FY24 SFWST milestone reports that were used to prepare the sub-sections of Section 6.

Table 6-1. A roadmap of sub-sections of Section 6 with cross-references to FY24 SFWT milestone reports.

Sub-sections of Section 6	DOE's Labs	Reports
6.1. Coupled Processes and Alterations in Bentonite-Based Engineered Barrier Systems		
6.1.2. Laboratory-Scale Experiments of Coupled Microbial-Abiotic Processes in Bentonite	LBNL	Zheng et al. (2024a, Section 5)
6.1.3. HotBENT High-Temperature Experiments and Modeling	LBNL	Zheng et al. (2024a, Sections 6 and 8)
6.1.4. Collaborative Modeling of the EBS Experiment at Horonobe URL	SNL	Jové-Colón and Lopez (2024, Sections 2, 3, and 4)
6.2. Experimental and Modeling Studies of Engineered Barrier and Host Rock Interactions		
6.2.2. Hydrothermal Experiments to Understand EBS and Host Rock Interactions	LANL	Rock et al. (2024a, Section 2) Rock et al. (2024b, Sections 2-4)
6.2.3. Bentonite Erosion, Coagulation/Flocculation, and Clogging	LANL	Viswanathan (2024, Section 1)
6.2.4. Modeling the CI-D Experiment at Mont Terri	LBNL	Rutqvist et al. (2024a, Section 9)
6.2.5. SKB Task Force (Task 12) Reactive-Transport Modeling of Cement-Bentonite Interactions	SNL LBNL	Carlos Jové-Colón, (2024, Section 5) Zheng et al. (2024a, Section 7)
6.3. Modeling of THM Processes in Heater Experiments in Argillaceous Rock		
6.3.2. Modeling of the FE Experiment in Opalinus Clay at the Mont Terri URL	LBNL SNL	Rutqvist et al. (2024a, Section 4) Hadgu et.al. (2024, Section 2)
6.3.3. Modeling of Thermal Fracturing in COx Claystone at the Bure URL	LBNL	Rutqvist et al. (2024a, Section 5)
6.4. Gas Migration in Clay-Based Materials: Modeling of the Field-Scale LASGIT Experiment		
6.4.2. Modeling of the LASGIT Experiment	LBNL	Rutqvist et al. (2024a, Section 10)
6.4.3. A New Interface Stability Model for Gas Channeling and Migration in Bentonite	SNL	Wang and Hadgu (2024, Section 2)
6.5. Modeling Coupled Processes, Fluid Flow, and Transport in Fractured Crystalline Rock		
6.5.2. Modeling Thermal Slip of Single Fractures	LBNL	Hu et al. (2024, Section 5)
6.5.3. Mechanical and Hydromechanical Simulations of a Single Fracture	SNL	Wang et al. (2024, Section 2)
6.5.4. Characterizing the Impact of Finite Matrix Block Size on Conservative Particle Transport	LANL	Viswanathan et al. (2024, Section 2)
6.5.5. A New Mesh Generation Methodology for Fracture Network Modeling	SNL	Hyman et al. (2024, Section 2)

Table 6-1 (continued). A roadmap of sub-sections of Section 6 with cross-references to FY24 SFWST milestone reports.

Sub-sections of Section 6	DOE's Labs	Reports
6.6. Salt Coupled Processes, Geomechanics, and Brine Migration		
6.6.2. International Collaboration through the RANGERS, KOMPASS, and MEASURES Projects	SNL	Mills et al. (2024, Sections 1 and 2)
6.6.3. Modeling of the Brine Availability Test in Salt	LBNL LANL	Rutqvist et al. (2024b, Section 5) Mills et al. (2024, Section 3) Guiltinan et al. (2023, Section 2)
6.6.4. NEA Salt Club	SNL	Mills et al. (2024, Section 5)
6.7. Hydromechanical Behavior of Faults in Response to Repository-Induced Perturbation in Argillite Rock		
6.7.2. Self-Sealing of Activated Faults in Argillite Host Rock	LBNL	Rutqvist et al. (2024a, Section 8)
6.7.3. Modeling Injection-Induced Fault Slip Using Long Short-Term Memory Networks	LBNL	Rutqvist et al. (2024a, Section 6)
6.8. Field-Scale Characterization of Fractures in Crystalline Rock		
6.8.2. Using 3D Displacement Measurements to Determine Stress State and Stress Heterogeneity	LBNL	Hu et al. (2024, Section 3)
6.9. Performance Assessment and Radionuclide Transport Modeling		
6.9.2. Comparative Performance Assessment Modeling of Crystalline and Salt Reference Cases	SNL	Mariner et al. (2024, Sections 2 and 3) LaForce et al. (2024, Sections 2-5) Mills et al. (2024, Section 3)
6.9.3. Thermodynamic and Thermochemical Database Development	LLNL	Zavarin et al. (2024a, Sections 2-5) Zavarin et al. (2024b, Sections 2-5)
6.10. Developing a Diverse Workforce for Radioactive Waste Disposal		
6.10.2. Overview of Workforce Development Activities at LBNL, SNL, and LANL	LBNL SNL LANL	Zheng et al. (2023) Mendez (2024) Caporuscio, 2023

6.1 COUPLED PROCESSES AND ALTERATIONS IN BENTONITE-BASED ENGINEERED BARRIER SYSTEMS

6.1.1 INTRODUCTION

Section 6.1 comprises summaries of SFWST's international modeling and experimental activities conducted in FY24 to improve the understanding of microbiological and temperature-induced perturbations and alterations in the EBS materials, focusing on bentonite as the principal buffer material. This section aims to highlight key findings as to how repository performance may be affected by THMC processes, perturbations, and alterations. The research activities described here are either aligned directly with the analysis and modeling of international field tests, such as the HotBENT Experiment and the Horonobe Experiment, or they use samples and materials from international programs and experimental efforts (e.g., FEBEX-DP).

Section 6.1.2 summarizes the results of laboratory-scale experiments conducted at LBNL to study coupled microbial-abiotic processes on bentonite samples collected during FEBEX-DP. Section 6.1.3 summarizes the ongoing experimental and modeling research related to the HotBENT laboratory and field experiments. These are designed to investigate whether a bentonite barrier can withstand temperatures exceeding 100°C and whether strongly elevated temperatures cause alterations compromising various engineered barrier functions and the host rock. Section 6.1.4 presents summaries of activities related to Task D of the international DECOVALEX-2023 Project; this section focuses on modeling the Horonobe EBS Experiment and includes supporting laboratory experiments conducted using a block of the Kunigel V1 bentonite used in the Japanese program.

6.1.2 LABORATORY-SCALE EXPERIMENTS OF COUPLED MICROBIAL-ABIOTIC PROCESSES IN BENTONITE

Background and International Connection: Bentonite samples that underwent different temperature regimes during the FEBEX *in-situ* experiment were tested to explore the possibility of microbial activity in bentonite materials (see Section 3.3.1 for a description of the FEBEX-DP project).

Objective: To investigate whether residual microbial communities can exist in bentonite emplaced in a heated, dry environment for an extended time and how they may be affected by long-term heating alterations. The FY24 effort aimed to complete the data analysis and prepare a manuscript for submission. No additional experimental work was performed.

Associated SFWST Milestone Report: Section 5 in Zheng et al. (2024), Engineered Barrier System R&D, LBNL Report, SF-24LB010308032.

Summary:

Studying coupled microbial-abiotic processes in bentonite is important because microorganisms are expected to survive in a nuclear waste repository and activate over time when gas is produced in the system, water penetrates through cracks in the host rock, or when other perturbations occur. In FY24, LBNL scientists finalized the analysis of laboratory experiments conducted on FEBEX bentonite samples. These samples were collected from different temperature zones in the heater test EBS--high heat, intermediate heat, and control zones. The objective was to test the hypothesis that even after long-term emplacement and exposure to elevated temperature, viable organisms capable of various metabolic processes, including H2 utilization, persist in the system.

The experimental results revealed that bentonite can sustain microbial communities with potential for growth. However, it was found that microbial communities did not grow in the hot zone during the experiment's time frame. Whether this lack of microbial growth is due to the heating, drying, or a combination of both remains to be determined. It was found that the specific communities were sensitive to gas composition and solid content changes. This tendency is supported by (a) the influence of high solid-to-solution ratios observed in one of the experiments and (b) the lack of significant microbial activity in the samples closest to the heaters. This study underscored the importance of observing non-H2 metabolism in fluids within the formation, which will help predict the dominant metabolic processes. Thus, the findings indicate the potentially significant role of microbial metabolism in long-term nuclear waste disposal repositories employing clayey materials as a barrier. Further research should explore the range of metabolisms possible within the barrier material's existing community and investigate how specific chemical and physical conditions regulate the microbial growth rate.

6.1.3 HOTBENT HIGH-TEMPERATURE EXPERIMENTS AND MODELING

Background and International Connection: The HotBENT field test is a full-scale high-temperature heater experiment conducted since 2020 at the Grimsel Test Site in Switzerland (see Section 3.3.2 for a description of the HotBENT Project). To support the interpretation and understanding of the field test, LBNL has been conducting a series of laboratory-scale experiments, named HotBENT Lab. Results from these experiments were utilized as a modeling task in the SKB EBS Task Force (see Section 3.4.3 for a summary of EBS Task Force activities).

Objectives: To investigate whether a bentonite barrier can withstand temperatures exceeding 100°C and to evaluate whether strongly elevated temperatures cause alterations compromising the engineered and natural barrier functions.

Associated SFWST Milestone Report: Sections 6 and 8 in Zheng et al. (2024), Engineered Barrier System R&D, LBNL Report, SF-24LB010308032.

Summary:

SFWST scientists continued participating in the HotBENT Project, with focus on interpreting and 3D modeling the full-scale field test and comparing it with the experimental data. In addition, the HotBENT-Lab #2 column experiment was continued to obtain well-characterized datasets that help understand the heating and hydration of bentonite.

- *Understanding the THMC Evolution of Bentonite Using Full-Scale Field Tests: HotBENT*

  The HotBENT field test progressed as planned in FY24: all the heaters had reached their respective target temperatures, and the heating phase continued at the design temperature. Data were collected through the extensive sensor network, and data from different sectors were shared with the partners. LBNL actively participates in the HotBENT Modeling Platform. LBNL's modeling studies of the HotBENT field experiment started using 2D TH modeling for a cross-section (Zheng et al., 2023a), which was then used to develop a 3D TH model. Later, the 2D TH model was expanded to a THM model. The 2D TH and THM model development was completed in FY24, and the 3D THM modeling is ongoing. The 3D TH model predictions match the trends observed in thermal and hydrodynamic behavior in the EBS. However, the current model underpredicts the temperature results in sectors surrounding the heaters with bentonite fill. The 2D THM model better captures the hydration behavior within the buffer, incorporating updated porosity introduced by the mechanical model.

  In FY25, LBNL will extend the 3D TH model to a 3D THM model which can be expanded to add chemical effects. This will help improve understanding of and provide information on the coupled THMC behavior of the EBS. To address the discrepancies with temperature and saturation predictions, efforts will be made to investigate the impact of different thermal conductivity functions (e.g., Lu and Dong, 2015), Soil Water Retention Curves (SWRCs), and mechanical constitutive models on the THM behavior of the EBS.

- *Heating and Hydration Column Test of Bentonite – HotBENT-Lab*

  During the planning stage of the HotBENT field test, HotBENT Lab #1 was conducted to support the field test design and scoping model calculation. It used Wyoming bentonite powder and hydrated at the 7 bars. Monitoring included XCT imaging to provide a 3D visualization of the density distribution changes due to water saturation, clay swelling, and structural deformation during the experiments. Temperature monitoring was conducted using thermocouples, and the ERT data were acquired using a DAS-1 electrical resistivity tomography (ERT) instrument and the electrical potential and chemical changes were monitored through effluent water and final mineralogical characterization. The spatiotemporal density distribution illustrates a dynamic interaction of the THM processes and the self-sealing of bentonite. The analyses after the columns were dismantled showed bentonite was primarily homogenized.

  HotBENT Lab #2 was conducted from FY23 to FY24 using the granulated Wyoming bentonite (30% powder and 70% pellets) received from the field test and hydrated with synthetic Grimsel groundwater at 2 MPa (the designed hydration pressure for the field test) and monitored using the same technique as the HotBENT Lab #1. However, the CT density showed distinct spatiotemporal distribution from HotBENT Lab #1, which indicates water flow through the powder first and hydrated the pellets secondary, a typical dual-continuum behavior.

  Research activities in FY25 will include additional analysis of the bentonites from HotBENT Lab #2 experiments. Also, a new column experiment, HotBENT Lab #3, will be conducted using the Czech bentonite provided by Nagra.

6.1.4 COLLABORATIVE MODELING OF THE EBS EXPERIMENT AT HORONOBE URL

Background and International Connection: Experimental and modeling activities were conducted under the DECOVALEX-2023 Project, Task D, which focused on the EBS Experiment at Horonobe URL. The Japanese waste management research organization JAEA led this task which has now ended (see synthesis of joint modeling results in Sugita et al., 2024). Section 3.2.2.4 provides a short description of DECOVALEX-2023 Task D.

Objective: The objective of this joint modeling activity is to understand better and be able to simulate the coupled THMC processes occurring in and around an engineered barrier system as designed in the Japanese disposal concept.

Associated SFWST Milestone Report: Sections 2 and 3 in Jové-Colón and Lopez (2024), International Collaboration Activities on Disposal in Argillite R&D: Characterization Studies and Modeling Investigations, SNL Report, SF-24SN01030108. The results presented in the SNL report should be considered the final Sandia's contribution to DECOVALEX2023 Task D, given the end of DECOVALEX-2023 project.

Summary:

DECOVALEX Task D was divided into two main steps. Step 1 aimed to test and demonstrate that international simulation models can handle the THM characteristics of bentonite as an engineered barrier material. This step comprises modeling laboratory experiments conducted by the JAEA to investigate the Kunigel V1 bentonite isothermal/non-isothermal saturation, swelling pressure, and free swelling. JAEA provided the experimental data to participating modeling teams. In Step 2, the knowledge gained from Step 1 was applied to build more complex models for simulations of the full-scale EBS Experiment, which was active from January 15, 2015, until March 31, 2022, for approximately 2,632 days. The field experiment involved a vertically emplaced overpack containing two heaters surrounded by buffer barrier material composed of silica sand and Kunigel V1 bentonite. SFWST researchers from SNL developed 1D PFLOTRAN models for two Step 1 experiments (S1-3 and S1-4), developed and applied a 2D model for the full-scale heater test, and compared their results with those of other international modeling groups.

- *1D Modeling of SI-3 and SI-4 Experiments*

  The S1-3 infiltration test conducted by JAEA examined the vertical saturation of a block of Kunigel V1 bentonite and silica sand for about 30 days. A 50 mm tall bentonite block was wetted from the bottom, and an air outlet was at the top. The wetting solution was either deionized water (DW) or 0.2 M NaCl aqueous solution as an analog for dilute groundwater (GW). The system was isothermal at ambient conditions and modeled at 25°C. The test assessed the saturation as a function of time and distance along the sample. The 1D PFLOTRAN 2-phase flow simulations of the S1-3 DW tests successfully represented the saturation profiles of the S1-3 experiment in Kunigel V1 bentonite and sand. However, initial saturation homogeneous vs. heterogeneous profiles primarily affect predicted saturation profiles at early times. The GW and DW simulations showed that the saturation experimental and modeling profiles are similar after one day of saturation. Overall, it was concluded that the 1D PFLOTRAN 2-phase flow model using two permeability zones can simulate the S1-3 bentonite isothermal saturation experiment, generating results in excellent agreement with the observed test saturation data.

  The SI-4 Experiment was conducted to study FEBEX bentonite hydration under non-isothermal conditions from 6 to 92 months (Villar et al., 2008a,b). These studies showed that thermal gradients could drive changes in the bentonite water content and dry density along the column length and could affect the permeability and swelling of bentonite (Villar et al., 2008b). Model predictions of liquid saturation using a uniform permeability tended to underpredict the S1-4 experimental data at the top of the sample. Preliminary data analysis indicated that changes in the permeability of the stratified bentonite regions have a much more significant effect on the resulting saturation profiles. Therefore, studies conducted in FY24 focused on parameter optimization in the simulation of the non-isothermal column experiments. It was shown that a 1D PFLOTRAN 2-phase TH flow model can simulate experimental results by using a stratified permeability approach represented by five permeability zones of the vertical bentonite column.

- *2D Modeling of the Full-Scale EBS Experiment*

  2D 2-phase TH simulations of the Full-Scale EBS Test at the Horonobe URL site were conducted using PFLOTRAN. The model description is given in Section 3 of Jové-Colón and Lopez (2024), and the 2D PFLOTRAN model domain is shown in Figure 12 of the report by Jové-Colón and Lopez (2024). The simulations have replicated essential temperature temporal trends for the duration of the heater test. With time, the simulated liquid saturation trend in the buffer shifts towards earlier times, when the predicted fast water vapor phase transport leads to fast resaturation. Even with this discrepancy, the overall behavior is considered representative of the system, showing a relatively fast recovery to full saturation upon heating initiation. The overall vapor transport rate from the simulation's buffer domain is relatively fast. However, the influence of water injection (around the buffer periphery) on buffer re-saturation and thermal gradients results in complex fluid flow behavior. The limitations of the 2D modeling domain and its spatial discretization necessitated adjusting the model inputs, such as the heater power and water injection rates. Also, PFLOTRAN cannot currently simulate the buffer mechanical behavior, such as bentonite swelling from water uptake and its coupled effects on porous media flow, thus limiting the physical representation of the problem. Still, the PFLOTRAN modeling of coupled two-phase flow under non-isothermal conditions is crucial to bentonite fluid mass and heat transport. Any future efforts should focus on 3D representations of flow in the system domain as well as to account for mechanical effects in the buffer material.

6.1.5 KEY ACCOMPLISHMENTS

- Collaborations with the international FEBEX-DP, HotBENT, and Horonobe EBS projects involve experimental and modeling studies to understand the effects of temperature-dependent perturbations and alterations in engineered barrier materials. These activities have provided valuable insights into how repository performance may be affected by these perturbations and changes.
- The post-mortem FEBEX-DP bentonite samples continue to provide a basis for evaluating potential EBS property changes. The results of laboratory-scale experiments investigating coupled microbial-abiotic processes in altered and unaltered bentonite samples indicate considerable metabolic potential within the microbial communities even after long-term exposure to heat. This is important because microorganisms that survive in a nuclear waste repository can later become active as gas is introduced or produced in the system, water is introduced through cracks in the containment or other environmental changes. This underscores the need to continue the study of microbial metabolism in long-term nuclear waste disposal repositories.
- The HotBENT field test has continued providing data on bentonite behavior at strongly elevated temperatures, which are now used for interpretative modeling. LBNL has developed a 3D TH model which is able to match the trends observed in the thermal and hydrodynamic behavior of the EBS. However, the current model underpredicts the temperature in the bentonite near the heaters. In FY25, LBNL will extend the 3D TH model to a 3D THM and possibly THMC model, which will improve the model predictions, especially when it comes to the buffer's hydration behavior.

- LBNL analyzed results from the HotBENT-Lab #2 column test, which used granulated Wyoming bentonite and lasted for 16 months. The laboratory experiment provides a unique data set of the spatio-temporal changes of bentonite affected by hydration, heating, and swelling.
- Modeling of the Horonobe EBS Experiment conducted in the framework of the DECOVALEX-2023 Task D demonstrated that the PFLOTRAN simulator can model two-phase flow under non-isothermal conditions, which is a crucial aspect of fluid mass and heat transport in the EBS. It was shown that a reduced order 2D model, instead of a full 3D model, can well represent the general temperature trends. Improvement of the 2D PFLOTRAN model is needed to simulate fluid flow affected by mechanical processes, such as bentonite swelling and related couplings with porous media flow. Ongoing research aims to improve the model setup to provide realistic field-scale test saturation behavior predictions.

6.2 EXPERIMENTAL AND MODELING STUDIES OF ENGINEERED BARRIER AND HOST ROCK INTERACTIONS

6.2.1 INTRODUCTION

This section summarizes SFWST's international activities to improve the understanding of physical and geochemical interactions between EBS and host rock materials. Material alterations near these interfaces can affect repository performance, for example, by changing the flow and transport of radionuclides through the engineered barriers into the surrounding natural rock. Interfacial reactions are most prominent early in a repository's lifetime when the EBS materials, such as bentonite, metal containers, and cementitious materials, have just been emplaced, and thermal-hydrological-mechanical-chemical perturbations remain strong. The results of experimental and modeling studies described in this section aim to provide insights into how interfacial processes and alterations, such as between different host rocks and EBS materials, may impact repository performance under strong THMC driving forces.

Section 6.2.2 summarizes results from hydrothermal laboratory experiments designed to study geochemical and mineralogical interactions between EBS and host rock components.

Section 6.2.3 includes results of experimental studies of bentonite erosion, coagulation/flocculation, and clogging in a fractured crystalline rock.

Section 6.2.4 provides reactive transport modeling results to interpret the evolution of the *in-situ* CI-D experiment at Mont Terri, which explores the long-term interaction between cement, bentonite, and Opalinus Clay.

Section 6.2.5 summarizes reactive-transport modeling activities conducted as part of Task 12 of the SKB EBS Task Force. The task is aimed at the comparative evaluation of reactive-transport models to represent interactions between bentonite and cement barrier materials.

6.2.2 HYDROTHERMAL EXPERIMENTS TO UNDERSTAND EBS AND HOST ROCK INTERACTIONS

<u>Background and International Connection</u>: LANL scientists conducted two types of experimental studies to understand better interfacial material alterations at conditions relevant to the EBS experiment at the Horonobe URL in Japan and the HotBENT experiment at the Grimsel Test Site in Switzerland:

(a) International collaboration with the Japan Atomic Energy Agency (JAEA) was initiated in FY21 to investigate the alteration of EBS and host rock materials at elevated temperature and pressure at the Horonobe URL. In FY24, LANL continued elevated-temperature laboratory experiments to simulate the conditions and materials of the full-scale EBS experiment at Horonobe.

(b) Hydrothermal experiments were conducted on granodiorite cores from the Grimsel Test Site in contact with EBS materials and exposed to synthesized GTS granodiorite groundwater to simulate bentonite alteration in a generic crystalline rock environment. These experiments used the same type of bentonite and a temperature range of up to 200°C as the HotBENT test. The experimental data help build the reactive transport model for the HotBENT field test (see Section 3.3.2 for more information on HotBENT).

Objectives: To characterize and quantify the effects of elevated pressure-temperature conditions on the mineralogical and geochemical characteristics of engineered barrier materials, which can be used to perform modeling of long-term EBS material stability.

Associated SFWST Milestone Reports: (a) Section 2 in FY24 reports by Rock et al. (2024a), Argillite International Collaborations, LANL Report, M3SF-24LA01030102, LA-UR-24-26106, and (b) Sections 2-4 in Rock et al. (2024b), Engineered Barrier System R&D and International Collaborations – LANL, SF-24LA01030801 & SF-24LA01030802, LA-UR-24- 29332.

Summary:

- *Hydrothermal Experiments at Conditions Relevant to Horonobe EBS Experiment*

  Elevated-temperature laboratory experiments were completed in FY24 (HNB-4 and -5) using Japanese Kunipia-F bentonite (powder) and low-carbon steel (LCS) with synthetic Wakkanai groundwater (WGW) from the Horonobe URL at 200°C and 150°C, respectively. The groundwater solution was prepared using reagent-grade materials dissolved in double-deionized water. NaOH and HCl were added to adjust the initial solution pH. The synthetic brine solution was added at the ~9:1 water: bentonite ratio. Initial components for wall rock experiments can be found in Table 1 of the report by Rock et al. (2024a). A comparison of the 150°C Kunipia-F to the 150°C Kunigel-V1 experiment indicates that both bentonites quickly approach a quasi-steady state chemical composition in contact with the Wakkanai groundwater. The experiments showed minimal alteration and may experience even less alteration for lower water-rock ratios.

  The HNB-5 experiment was conducted using low-carbon steel (LCS), one of the candidate materials for waste disposal. The experiment resulted in minor Fe leaching of the LCS, but no pitting or crevice corrosion was observed. The Fe content in the smectite in contact with the steel decreased with distance from the steel surface, suggesting that the effects of the steel are highly localized and restricted to the steel-bentonite interface. No Fe-rich phyllosilicates were observed in HNB-5. Minor general corrosion is the most likely mechanism to occur in repository conditions.

- Hydrothermal Experiments at Conditions Relevant to HotBENT

  Two experiments in FY24 included Wyoming bentonite (used in the area around Heaters #1, #2, and #3 in the HotBENT field test) or Czech bentonite (BCV, used to backfill the area around Heater #4 in the HotBENT) + low carbon steel + Grimsel granodiorite synthetic groundwater, reacted at 200°C and 150 bar for eight weeks. Together with three additional experiments about bentonite (Wyoming and BCD) + low-pH cement + Grimsel granodiorite synthetic groundwater, five experiments were completed from FY23 to FY24.

  Hydrothermal experimental studies showed that montmorillonite remained stable at 250°C, indicating that the relatively K-poor bulk composition of the system likely prevented smectite illitization. Wyoming bentonite showed no substantial alteration of the montmorillonite to secondary non-swelling clay phases at experimental conditions. The alteration of the swelling clay montmorillonite to non-swelling illite (illitization) in Wyoming bentonite in a Grimsel granodiorite wall rock environment is interpreted to be restricted due to the bulk geochemistry of the overall system (i.e., low K) and/or kinetics. Preliminary findings suggest that the clay barrier material (Wyoming bentonite) may only experience slight alteration in the initial thermal pulse in a repository setting. These findings will be compared to results after the initial and final stages are completed of the long-term, full-scale demonstrations (HotBENT).

These results will be incorporated into a database of Grimsel granodiorite and EBS experiments for use in evaluation of EBS materials performance at elevated temperatures in crystalline environments. The mineralogical and geochemical changes observed in the Wyoming bentonite-Grimsel granodiorite experiments can be applied to understanding potential material interactions in a high-temperature, crystalline repository.

6.2.3 BENTONITE EROSION, COAGULATION/FLOCCULATION, AND CLOGGING

Background and International Connection: LANL researchers have continued to collaborate with international partners to investigate the effects of colloid aging on the colloid-facilitated transport of radionuclides. This work is loosely connected with international collaboration efforts conducted with the CFM Project (i-BET experiment). The CFM project conducts radionuclide migration experiments in a fracture shear zone in the GTS. It is complemented by laboratory and modeling studies (see Section 3.3.3.3 of this report for more information on CFM).

Objective: Perform experiments to study bentonite clay erosion, coagulation/flocculation, and simulated fracture clogging behavior under controlled conditions.

Associated SFWST Milestone Report: Section 1 in Viswanathan et al. (2024), Crystalline and Crystalline International Disposal Activities, LANL Report, M4SF-23LA010302.

Summary:

Experiments were designed to study bentonite clay erosion, coagulation/flocculation, and fracture clogging behavior under controlled conditions. The experiments were conducted using unwashed Wyoming-Ben Big Horn 325 bentonite, a non-treated sodium bentonite in either an uncompacted, compacted, or colloidal form. Methods were developed for assembling an experimental apparatus, developing measurement techniques, and optimizing experimental conditions. These experiments consisted of a bentonite erosion cell and a bentonite coagulation cell. Results from the bentonite erosion experiments suggest that temperature could play an essential role in the combination of erosion and coagulation processes, which govern the behavior of bentonite colloids from a performance assessment perspective. Future work will focus on developing a single experimental system to study erosion and coagulation in one experiment. Future experiments will be conducted using washed and homoionic forms of bentonite and hydrothermally aged/altered bentonite to determine the parameters impacting the bentonite erosion and coagulation in geochemical conditions relevant to spent nuclear waste repositories, as well as the effect of the emplacement pressure (i.e., the initial pressure to which the bentonite plug is subjected).

6.2.4 MODELING THE CI-D EXPERIMENT AT MONT TERRI

Background and International Connection: The CI-D experiment at the Mont Terri URL focuses on the long-term (>15 years) interaction between cement, bentonite, and Opalinus Clay (see Section 3.1.4). LBNL's model simulates the hydro-chemical couplings occurring during the CI-D experiment using the code CrunchClay, an evolving branch of the CrunchTope/CrunchFlow family of simulators (Steefel et al., 2015).

Objective: Perform hydro-chemical modeling studies to interpret the observed evolution of the CI-D experiment at Mont Terri, focusing on understanding the reaction-induced porosity, permeability, and diffusivity changes in both the cement and the Opalinus Clay because of their interaction.

Associated SFWST Milestone Report: Section 9 in Rutqvist et al. (2024a), Investigation of Coupled Processes in Argillite Rock: FY24 Progress, LBNL Report, M3SF-24LB010301032.

Summary:

Simulations of the CI-D diffusion test at Mont Terri were conducted using 1D radial, 2D axisymmetric, and 3D full dual-continuum numerical models using LBNL's CrunchClay software, which considers electrostatic effects in the Opalinus Clay with complex electrical double layer models (Tournassat and Steefel, 2019; Tournassat et al., 2020; Steefel and Tournassat, 2021). The 1D radial and 2D-axisymmetric models included only the cement and were used to estimate diffusion coefficients in the cementitious material. However, of these two models, only the 2D-axisymmetric model provided reasonable results. A 3D model was developed and applied to simulate tracer transport for 450 days, and the results were compared favorably with the 2D-axisymmetric model. These simulations use the full dual continuum model in CrunchClay, which considers electrostatic effects in the electrical double layer (EDL). However, these effects are not readily apparent in the simulations because of the limited duration of the simulation time; the plume does not extend significantly into the Opalinus Clay by this time. Additional runs will be needed to extend it to the time scale of the experiment. The next step is to incorporate more complex geochemistry for the cement and the Opalinus clay, such as a rigorous treatment of mineral dissolution, precipitation, and sorption. This will allow a direct comparison between the simulation results and the data derived from the planned overcoring of the cement-claystone interface of the CI-D experiment, expected to be completed later in 2024.

6.2.5 SKB TASK FORCE (TASK 12) REACTIVE-TRANSPORT MODELING OF CEMENT-BENTONITE INTERACTIONS

Background and International Connection: Reactive transport modeling of cement-bentonite interactions is conducted as Task 12 of the SKB EBS Task Force. Results for collaborative modeling of a stylized benchmark problem are compared between four modeling teams: SKB, SURAO, LBNL, and SNL. See Section 3.4.3.2 of this report for more information on Task 12 of the EBS Task Force.

Objective: Evaluate and test reactive-transport models to represent interactions of backfill bentonite and cement barrier materials using a benchmark problem with different levels of complexity. The test of modeling approaches is based on comparison between various modeling groups.

Associated SFWST Milestone Reports: (a) Section 4 in Jové-Colón and Lopez (2024), International Collaborations Activities on Disposal in Argillite R&D: Characterization Studies and Modeling Investigations, SNL Report, M3SF-24SN01030108, and (b) Section 7 in Zheng et al. (2024), Engineered Barrier System R&D, LBNL Report, SF-24LB01030803.

Summary:

Task 12 was divided into three subtasks: Subtask A simulates the interaction between OPC and MX-80 bentonite under fully saturated conditions; Subtask B simulates the interaction between low pH concrete (LPC) and MX-80 under different initial saturation conditions; and Subtask C is to simulate the interaction between OPC and MX-80 with different initial and boundary conditions (e.g., unsaturated conditions). Researchers from SNL and LBNL participated in this modeling task together with two other international modeling groups. Reactive transport modeling for the concrete/bentonite interaction is complex, and benchmarking is challenging; many aspects of the model development include conceptual model choices such as selection of the thermodynamic database, kinetic reaction rate, selection of aqueous complexes, and choice of secondary minerals. While the task force tried to harmonize these aspects, each team was allowed to make their choice.

- *SNL 1D Reactive-Transport Modeling of Cement-Bentonite Interactions*

  This work builds on SNL initial modeling work reported in FY22 (Jové-Colón et al., 2022) and FY23 (Jové-Colón and Lopez, 2023). The modeling studies comprise a rectangular domain of fully saturated MX-80 bentonite and OPC domain, interacting for 100,000 years. The domains are isothermal at 25°C and held at constant atmospheric pressure. In Subtask A, the concrete domain comprises OPC, whereas in Subtask B, it is made of LPC. Modeling was conducted using

PFLOTRAN (Lichtner et al., 2019), with the application of the THERMODDEM database (Blanc, 2017; Blanc et al., 2012) and the addition of specific cement phases from CEMDATA18 (Lothenbach et al., 2019).

Task 12 Subtask A (OPC): The PFLOTRAN 1-D reactive-transport model of cement-bentonite interactions shows significant changes in spatial-temporal concentration profiles for Ca and Si at early times near the interface. The influence of pore solution chemistry in the domain with the largest saturated porosity (bentonite) affects the diffusive fluxes between domains and the long-term evolution of pore solution chemical composition across all domains. The most active solid in the simulations is gypsum, particularly at the interface region. Ettringite saturates in the OPC region.

Task 12 Subtask B (LPC): Like in subtask A, large concentration variations of Ca and Si were observed until ~100 years. Afterward, their concentrations stabilize to the levels of the bentonite pore solutions. The pH evolution in LPC differs from the OPC in subtask A, where it decreases to circum-neutral values at later times after a significant increase at early times. As with subtask A, pore solution chemistry in the domain with the largest saturate porosity affects diffusive fluxes and long-term pore solution chemical behavior.

Task 12 Subtask C (OPC and unsaturated bentonite): The initially unsaturated bentonite region reaches saturation in ~20 years by a front moving away from the saturated OPC interface. The saturation front in the bentonite controls the pore solution chemistry. In subtasks A and B, most changes in pore solution concentrations of Ca, Si, and pH occur near the interface because of the most significant solute concentration gradient. When the bentonite region becomes saturated with time, pH increases significantly. In the long term, total Ca and Si concentrations are comparable to those in the OPC region.

Future work will include continuing 1D PFLOTRAN reactive-transport modeling of Subtask C and evaluating parameter sensitivity on boundary conditions to assess code run stability issues and effects on diffusive fluxes.

- *LBNL Modeling of the Mineral Alterations at the Cement-Bentonite Interface*

  LBNL set up a TOUGHREACT model for the Task 12 modeling challenge and conducted simulations for Subtasks A1, A2, and A3, and B1, B2, and B3. In Subtask A, where interaction between MX-80 bentonite and OPC occurs, areas with significant mineral alteration are limited to 5-10 cm next to the interface. On the OPC side, porosity drops to almost zero in the area 3-5 cm away from the interface; on the MX-80, porosity increases to as high as 0.7, about 62% higher than the initial porosity of 0.43. Mineralogical changes in OPC are characterized by the dissolution of portlandite, C3AH6, monocarboaluminate, and CSH1.6 and the precipitation of ettringite, hydrotalcite and the appearance of CSH1.2, phillipsite, stratlingite and brucite. Mineralogical changes in MX-80 include the dissolution of gypsum, calcite, montmorillonite, illite, and quartz and the precipitation of K-feldspar, clinochlore, muscovite, analcime, heulandite-Ca, heulandite-Na, kaolinite and saponite. Modeling results for Subtask A are not sensitive to the initial porewater composition.

  In Subtask B, for interaction between MX-80 and LPC, areas with significant mineral alteration are limited to 5-10 cm next to the interface. OPC experienced a substantial drop of porosity (to almost zero) in the area 1 cm away from the interface but an increase in porosity in an area further away from the interface; MX-80 has the most significant porosity of 0.47 right next to the interface, only 9% higher than the initial porosity of 0.43. Mineralogical changes in OPC are characterized by the dissolution of SiO_2(am), CSH0.8, katoite, and precipitation of hydrotalcite and thaumasite. Ettringite precipitates until 10,000 years but then dissolves in the area about 10 cm away from the interface. Mineralogical changes in MX-80 include the dissolution of gypsum, calcite, montmorillonite, illite, and quartz and the precipitation of K-feldspar, clinochlore, muscovite, analcime, heulandite-Ca, heulandite-Na, Kaolinite and saponite. Model results for Subtask B are not sensitive to the initial porewater composition. Subtasks B1, B2, and B3 lead to similar results in the long run.

Above predictions on the alteration of the mineral phase around the interface area may significantly change the porosity and subsequently permeability, and, therefore, can have a profound impact on the long-term migration of radionuclides through bentonite buffer. In FY25, LBNL will continue modeling and sensitivity analysis of the participating teams' Task 12 results, with the goal of establishing a 'standard' practice for reactive transport modeling of bentonite.

6.2.6 KEY ACCOMPLISHMENTS

- Hydrothermal laboratory experiments were conducted to understand better interfacial material alterations at conditions relevant to the EBS experiment at the Horonobe URL in Japan and the HotBENT experiment at the Grimsel Test Site in Switzerland.
  - The experiments related to Horonobe conditions conducted on two different bentonites at 150°C demonstrated that these remained relatively stable and did not undergo extensive alteration in the presence of the Wakkanai groundwater. The chemistry of the aqueous phase between the two bentonites showed little difference, and there was no evidence of the transformation of the smectite to illite or another phyllosilicate.
  - The hydrothermal experiments on Wyoming bentonite-Grimsel granodiorite samples similarly showed that montmorillonite remained stable at high temperatures, indicating that the relatively K-poor bulk water composition of the granitic host rock likely prevented illitization. These findings suggest that the clay barrier material (Wyoming bentonite) may only experience slight alteration in the initial thermal pulse in a repository setting.

  The mineralogical and geochemical changes observed in both experimental settings can be applied to develop conceptual and numerical models for assessing long-term material stability in a high-temperature repository. The database of reacted EBS materials, along with conclusions of alteration of EBS materials in a rock environment similar to Horonobe, will be useful to experimental teams, modeling groups, and the international repository science community.

- Experiments were conducted to study bentonite clay erosion, coagulation/flocculation, and fracture clogging behavior under controlled conditions. Results demonstrated the need for a new experimental setup to study erosion and coagulation from a single experimental system because a combination of erosion and coagulation will ultimately govern colloid transport. Future experiments will be conducted using washed and homoionic forms of bentonite versus hydrothermally aged/altered bentonite to understand the parameters that significantly impact bentonite erosion and coagulation in geochemical conditions relevant to nuclear waste repositories. This work is loosely connected to international collaboration efforts conducted in the CFM project.
- Reactive transport simulations were conducted to interpret interfacial reactions and their impact across aged bentonite, concrete/cement, and clay rock interfaces. These activities were aligned with (1) the international CI-D experiment, which probes diffusive transport across materials emplaced in a borehole at the Mont Terri URL, and (2) the reactive-transport modeling of cement-bentonite interaction as part of the SKB EBS Task Force Task 12 benchmarking activities:
  - Simulations of the CI-D cement-clay interaction test at Mont Terri using the CrunchClay software, which considers electrostatic effects in the EDL models, demonstrated the need to extend the duration of modeling and use a more comprehensive reaction network to predict long-term cement and cement-clay interactions.

- The Task 12 benchmarking of geochemical changes due to cement-bentonite interaction showed substantial changes in pore solution chemistry, particularly at early times. This can lead to considerable alteration of highly soluble minerals, which can significantly change the porosity and permeability near the interface, possibly impacting the long-term migration of radionuclides through a cement-bentonite EBS. However, the simulations also demonstrated that areas with strong mineral alteration are limited to a few cm next to the interface. Future work will evaluate the safety implications of these complex interfacial alterations.

6.3 MODELING OF THM PROCESSES IN HEATER EXPERIMENTS IN ARGILLACEOUS ROCK

6.3.1 INTRODUCTION

Section 6.3 summarizes R&D activities related to the modeling of THM processes observed in large-scale *in-situ* heater experiments conducted in argillaceous rock. These experiments emphasize the argillaceous host rock rather than the EBS as emphasized in Sections 6.1 and 6.2.

The international activities described below have been performed to validate models of THM processes in claystone rocks for two repository design emplacements: (a) horizontal tunnels with bentonite backfill (Swiss concept) and (b) horizontal micro-tunnels extending from the walls of access tunnels (French concept). Sub-section 6.3.2 summarizes the THM modeling of the full-scale FE Experiment at the Mont Terri URL in Switzerland. Sub-section 6.3.3 summarizes the THM modeling of the CRQ Thermal Fracturing Experiment at the Bure URL in France. Both modeling activities have been conducted under the umbrella of the DECOVALEX-2023 initiative, which ended this fiscal year.

6.3.2 MODELING THE FE EXPERIMENT IN OPALINUS CLAY AT THE MONT TERRI URL

Background and International Connection: The full-scale emplacement experiment (FE experiment) at the Mont Terri URL was designed to replicate the emplacement tunnel of Nagra's reference repository design at a 1:1 scale as an ultimate test for the PA of geologic disposal in Opalinus Clay (OPA). Monitoring data from this test served as the basis for the DECOVALEX-2023 Task C modeling, which allows for model-to-model and model-to-data comparison of multiple approaches to simulating the THM response of the EBS and the host rock. See more details on the FE Heater Test in Section 3.1.2 and DECOVALEX-2023 Task C in Section 3.2.2.3 of this report.

Objective: To model the full-scale FE heater experiment at Mont Terri, including benchmarking, design predictions, and interpretative modeling. This task sought to understand pore pressure evolution in the host rock and how this is affected by heating, engineering factors (e.g., shotcrete, tunnel shape), and damage due to tunnel construction and thermal effects.

Associated SFWST Milestone Reports: (a) Section 4 in Rutqvist et al. (2024a), Investigation of Coupled Processes in Argillite Rock: FY24 Progress, LBNL Report, M3SF-24LB010301032, and (b) Section 2 in Hadgu et al. (2024), Engineered Barrier System International Collaborations, SNL Report M4SF-23SN010308062.

Summary:

Researchers from SNL and LBNL participated in Task C together with eight other international modeling groups. The task was structured into several steps, starting with a preparation and benchmarking phase (Step 0), followed by modeling of the FE heating phase (Step 1), and finally modeling of the FE ventilation phase (Step 2). In FY24, both LBNL and SNL teams were finalizing the Task C work, wrapping up Step 1 and Step 2 work, and publishing relevant findings from the comparative modeling activities.

- *THM Modeling of the FE Heater Test at LBNL*

  THM Modeling of the Mont Terri FE heating experiment, including benchmarking, heating design simulations, model predictions, and interpretative modeling, was performed at LBNL based on field data collected for five years of heating. Using TOUGH-FLAC, the host rock is modeled as an anisotropic medium, considering the bedding planes of the OPA. To accurately represent anisotropic thermal and hydrological behavior, a TOUGH2 inclined mesh was created. The benchmarking of the 2D THM model resulted in a good agreement between the teams. After obtaining a good match for the benchmark testing, the teams modeled the full-scale experiments using 3D model domains. Modeling the FE experiment indicates that the excavation-induced damage in the rock might significantly impact the heating-induced pore pressure increase and its dissipation. The properties and extent of damaged OPA around tunnels have yet to be studied in detail to capture the pore pressure in the OPA. A sensitivity study showed the need for modeling using reduced permeability and increased fluid storage. The best overall match was achieved by modeling an anisotropic permeability of 5×10^{-20} m^2 parallel to bedding and 1×10^{-21} m^2 perpendicular bedding, while the storage was increased by setting the pore compatibility at 2×10^{-9} Pa^{-1}. Future research will include model calibration, simulations of the concrete liner and EDZ, and modeling of the stress in the bentonite buffer.

- *TH Modeling of the FE Heater Test at SNL*

  SNL conducted TH modeling for Steps 1 and 2 of DECOVALEX-2023 Task C. The 3D modeling of the experimental tunnel was performed for a cylindrical tunnel model with heaters placed in the tunnel centerline. In the model, the Opalinus Clay host rock is bedded and anisotropic in directions parallel and perpendicular to the bedding plane that dips 34° from the horizontal. The model domain of 50 m x 50 m x 50 m was used for TH simulations with different mesh sizes. Step 1 involved modeling the heating phase of the FE experiment with changes in pore pressure in the Opalinus Clay. The PFLOTRAN (Hammond et al., 2014) numerical model calibration was conducted using a 5-year observational dataset of temperature, pressure, and relative humidity at various locations. Hydraulic properties were calibrated based on the equation-of-state from the International Formulation Committee (1997). The objective of Step 2 was to refine the models representing the FE experiment using additional data, starting from the ventilation phase and continuing to the heating phase. For this phase, the SNL team added a representation of the ventilation of the FE tunnel before backfilling, followed by shotcrete lining of the tunnel and backfilling. Experimental data from the ventilation period were used to calibrate the 3D model further and generate initial conditions for the heating phase. Calibrations of the ventilation and heating phases in Step 2 refined the model generated in Step 1.

Collectively, the international teams involved in Task C of DECOVALEX-2023 were able to simulate the THM coupled processes relevant to the FE experiment and successfully reproduced the data (see Task C synthesis paper by Graupner et al., 2024). Those results for the FE experiment were only achieved due to the rather extensive benchmark studies conducted beforehand. This underlines the value of well-constrained benchmarking studies when comparing complex process model implementations.

6.3.3 MODELING OF THERMAL FRACTURING IN COX CLAYSTONE AT THE BURE URL

Background and International Connection: The CRQ experiment at the Bure URL has been designed to test the behavior of COx claystone exposed to a thermal fracturing stress regime by reproducing the evolution of pressure, temperature, and stress in the HLW repository. Comparative THM modeling was conducted under the umbrella of Task A of the DECOVALEX-2023 Initiative (Section 3.2.2.1).

Objectives: To improve the ability of THM models to predict the processes and mechanisms of fracture initiation and growth in claystone due to a rapid increase in thermal overpressure.

Associated SFWST Milestone Report: Section 5 in Rutqvist et al. (2024a), Investigation of Coupled Processes in Argillite Rock: FY24 Progress, LBNL Report, M3SF-23LB010301032.

Summary:

Researchers from LBNL participated in Task A of DECOVALEX-2023 together with several other international modeling groups, using a variety of conceptual and numerical approaches to simulate thermal hydrofracturing. LBNL used the TOUGH-FLAC simulator for the coupled THM simulation of the *in-situ* heating experiment model (Rinaldi et al., 2021; Rutqvist, 2011). This simulator combines TOUGH3 and FLAC3D, which are thermo-hydraulic and mechanical modeling software, respectively, and couples them in a sequential scheme. Contrary to the linear elastic model reported in the FY23 progress report, in FY24, the thermal hydrofracturing was simulated using an anisotropic mechanical model. The THM-coupled modeling using mechanical constitutive models for the COx weak planes to simulate formation bedding enabled accurate predictions of fracture development and fracture locations. LBNL then used the improved model to examine the effects of (i) the weak planes, (ii) the softening rate of matrix/weak plane strength, and (iii) the stiffness anisotropy of the COx on the development of shear and tensile fractures during heating. As observed in the diagonal directions, the COx stiffness anisotropy significantly affected fracture development, including shear fracture development. Fracture development intensified at a threshold softening rate of rock strengths while using an insignificant or zero softening rate, which predicted only a few fractures. The results of 3D TH modeling of the CRQ experiment matched the observed pore pressure and temperature changes. These results have been summarized in the journal paper by Sasaki et al. (2024). However, this research did not consider the complex interaction between rock failure and permeability, as the permeability was assumed constant. In future research, the effect of such complex interaction will be investigated to improve the prediction of fracture development in the COx during heating generated by radioactive waste.

LBNL's predictions, along with those from other international teams, demonstrated that a portfolio of different THM modeling approaches was able to analyze and reproduce fracture initiation in the COx in terms of time of occurrence and location based on their respective stress analyses (Plúa et al., 2024a). However, attempts to reproduce fracture aperture or fracture propagation were less accurate and require more work in the future.

6.3.4 KEY ACCOMPLISHMENTS

- The full-scale FE heater test at Mont Terri, now in its 10th year of heating, continues to provide valuable THM data at relevant spatial and temporal scales. Under the umbrella of Task C of the DECOVALEX-2023 project, SFWST researchers and several international partners worked on interpretative and comparative THM simulations for model validation. Based on a comprehensive sensitivity study, the teams were able to achieve an excellent overall match with the measured pore pressure changes in the host rock when considering reduced near-field permeability and increased fluid storage. After completing the work with DECOVALEX-2023, LBNL will resume regular Mont Terri project simulations of the 10-year field data at the FE Experiment. The work for the Mont Terri project will focus on the interaction of the host rock with the bentonite buffer and the stress in the bentonite buffer.
- The ability to simulate processes and mechanisms of thermal fracture initiation was tested in Task A of the DECOVALEX-2023 project. Modeling of the CRQ *in-situ* heating experiment showed that different THM modeling approaches were able to reproduce fracture initiation in the COx in terms of time of occurrence and location whereas attempts to reproduce fracture aperture or fracture propagation were less accurate and require more work in the future.

6.4 GAS MIGRATION IN CLAY-BASED MATERIALS: MODELING OF THE FIELD-SCALE LASGIT EXPERIMENT

6.4.1 INTRODUCTION

This section summarizes SFWST's FY24 activities aimed at modeling of gas migration in compacted bentonite using the data collected at the LASGIT field experiment, according to Task B of DECOVALEX-2023. LASGIT is a full-scale gas injection experiment conducted at a 420 m depth in the Äspö Hard Rock Laboratory, Sweden, to examine the processes controlling gas and water flow in water-saturated and highly compact buffer bentonite, which are related to the Swedish KBS-3 repository concept (Cuss et al., 2014). An overview of the test is given in Section 3.2.2.2. A mockup waste canister (without a heater) was placed in a deposition hole drilled into the gallery floor, which was then filled with pre-compacted bentonite blocks. 13 circular filters of varying dimensions were placed on the surface of the canister to provide point sources for the injection of gas, which would then migrate through the bentonite toward the crystalline host rock. Section 6.4.2 summarizes the results of collaborative modeling of the LASGIT Gas Test 4. Section 6.4.3 describes the development of a new theoretical model for gas channeling and migration in compacted bentonite. The DECOVALEX-2023 phase has now ended, and the Task B modeling work has wrapped up with the publication of two synthesis papers co-authored by the participating research teams (Tamayo-Mas et al., 2024a,b).

6.4.2 MODELING OF THE LASGIT EXPERIMENT

Background and International Connection: Gas migration modeling has been conducted according to Task B of the DECOVALEX-2023 Initiative. This task aims to improve understanding of processes and mechanisms governing the advective movement of gas in compacted bentonite, improve physics-based models of these systems, and support the development of performance and safety assessment models. See more details on DECOVALEX-2023 Task B in Section 3.2.2.2 of this report.

Objective: To perform collaborative modeling of the LASGIT Gas Test 4 and compare simulated and measured flow rate, pressure, and stress responses at different monitoring points.

Associated SFWST Milestone Report: Section 10 in Rutqvist et al. (2024a), Investigation of Coupled Processes in Argillite Rock: FY24 Progress, LBNL Report, M3SF-23LB010301032.

Summary:

LBNL's approach to gas migration modeling features a 3D TOUGH-FLAC continuum model with multiphase (gas and liquid) flow, a linear poroelastic model, a linear moisture swelling model, and a gas permeability model related to minimum effective compressive stress. For DECOVALEX-2023 Task B, LBNL used this approach first for some collaborative benchmarking and blind predictions of laboratory-scale experiments. The analysis and results of these activities were summarized in the report by Rutqvist et al. (2024a) and a recently published synthesis paper by Tamayo-Mas et al. (2024a).

In FY24, HM modeling of the LASGIT Gas Test 4 was performed with the same modeling approach as was applied for the modeling of benchmarks and laboratory experiments, but with the consideration of interfaces between the canister and bentonite blocks, between individual bentonite blocks, and between the bentonite and host rock. LBNL's simulation results featured a good comparison between simulated and experimentally determined pressure and injection flow rate. These results also showed how the injected gas propagates preferentially along interfaces between the bentonite and host rock, which is consistent with field observations from LASGIT (Cuss et al., 2022).

A comparison of simulation results and monitoring data related to the LASGIT experiment is presented in the synthesis paper by Tamayo-Mas et al. (2024b), based on the predictions of multiple international modeling teams such as BGR/UFZ, LBNL, UPC/Andra, and KAERI using different codes such as OpenGeoSys, TOUGH-FLAC, and COMSOL. The teams applied the models developed and validated against the laboratory tests without substantial modifications, except for adding interface between bentonite blocks to reflect the experimental configuration of LASGIT and adjusting the bentonite permeability. The modeling results from the teams showed a reasonable agreement with each other and with experimental data such as the measured gas pressure and gas injection volume (Tamayo-Mas et al., 2024b). The fact that these updated models were able to represent most of the key features observed in the experimental data, even at a large scale, adds confidence to the prediction of repository-scale gas migration for performance assessment.

6.4.3 A NEW INTERFACE STABILITY MODEL FOR GAS CHANNELING AND MIGRATION IN BENTONITE

Background and International Connection: Laboratory and field experiments of gas migration in low-permeability deformable clay or bentonite materials have consistently exhibited chaotic patterns of channelized flow and high-frequency fluctuations of gas influx and outflux. A new nonlinear modeling approach has been developed that can account for such channelized chaotic gas flow and can be upscaled, e.g., to support the gas migration modeling conducted under the umbrella of Task B of the DECOVALEX-2023 Initiative (Section 3.2.2.2).

Associated SFWST Milestone Reports: Section 2 in Wang and Hadgu (2024), Year-end Report on International Collaboration on Spent Fuel Disposal in Crystalline Rocks, SNL Report, M4SF-24SN010302082.

Objective: To demonstrate that the observed complex behaviors of gas percolation in low-permeability bentonite materials can emerge from the morphological instability of the interface between the gas phase and the material matrix, and to develop a new model of gas channeling and migration in water-saturated compacted bentonite based on the theory of linear stability.

Summary:

Based on the theory of the linear stability analysis, SNL scientists demonstrated that gas channeling can autonomously emerge from the morphological instability of the interface between the injected gas and the compacted bentonite due to local stress concentration, pore dilation, and hydrologic gradient variation. Channel patterns can be described using a model of fractal geometry, which provides a new perspective for upscaling the process from small scale laboratory observations to a field scale. Once a percolating channel is established, the gas injected would percolate through the channel as a chain of gas bubbles, resulting in the interface instability, and aperiodic/chaotic variations in gas flow rate (Faybishenko et al., 2021).

To better understand the physical mechanisms involved in these processes, Wang and Hadgu (2024) provided a new theoretical model for the complex mechanism of nonlinear dynamics of gas migration in water-saturated compacted bentonite. The new model accounts for channelized gas migration as well as both morphological and hydrological instabilities at the gas-bentonite interface. It can represent the observed complex migration patterns with rapid breakthrough, periodic/chaotic gas flux, fast percolation, and low gas saturation. Thus, the concept and the models developed in this work predict the key features observed in gas injection experiments and portray a quite different picture for gas percolation in low-permeability deformable media than that traditionally conceived from permeable porous media. Although the theoretical framework of the linear stability analysis provides a new perspective for model development and simulations of gas percolation in low-permeability deformable media, this approach has certain limitations: it is limited to 2D systems, the model analysis does not consider nonlinear processes, and only simplified boundary conditions for modeling are considered. Future work should be focused on relaxing these limitations.

6.4.4 KEY ACCOMPLISHMENTS

- Under the umbrella of Task B of the DECOVALEX-2023 project, SFWST scientists and their international partners tested their predictive capabilities for gas migration against data from the full-scale LASGIT experiment conducted at the Äspö Hard Rock Laboratory in Sweden. LBNL scientists were able to show that an HM modeling approach that was initially developed to simulate small-scale gas injection laboratory experiments could be extended to match the LASGIT field observations.
- A new conceptual model was developed to best capture the complex phenomenological behavior of gas flow through bentonite. The new model can represent observed gas migration patterns such as rapid breakthrough, aperiodic/chaotic gas flux, fast percolation, and low gas saturation. Due to fractal scale invariance, this may provide a new perspective for upscaling from small scale laboratory observations to a field scale. Based on the theory of the linear stability analysis, it was shown that gas channeling can emerge from the morphological instability of the interface between the injected gas and the compacted bentonite due to local stress concentration, pore dilation, and hydrologic gradient variation.

6.5 MODELING COUPLED PROCESSES, FLUID FLOW, AND TRANSPORT IN FRACTURED CRYSTALLINE ROCK

6.5.1 INTRODUCTION

Investigations of crystalline rock formations as host rock for radioactive waste disposal have been conducted throughout the world (e.g., Sweden, Korea, Japan, Canada, China) and have been studied at several URLs, for example at the Äspö HRL in Sweden and at the GTS in Switzerland. The most advantageous features of crystalline/granite rock concerning radioactive waste isolation are mechanical stability, low permeability, and high thermal conductivity. However, because crystalline formations are often fractured, repository performance assessment studies require an understanding of (1) the characteristics and properties of existing fracture networks, (2) the impact of stress changes and other perturbations on these fracture networks, and (3) the large-scale transport patterns of radionuclides migrating in fracture networks from the repository to the biosphere.

Sections 6.5.2 and 6.5.3 summarize the results of TM and HM modeling studies of single fracture response to thermal and mechanical stresses conducted in the framework of DECOVALEX-2023 Task G, which utilized novel laboratory-scale experiments that link micro-scale effects acting on fracture surfaces with emergent fracture properties such as permeability. The DECOVALEX-2023 task has now ended, and the Task G modeling work has wrapped up with the publication of a synthesis papers co-authored by the participating research teams (Kolditz et al., 2024).

Sections 6.5.4 and 6.5.5 summarize SFWST modeling efforts related to Task 10 of the SKB GWFTS Task Forces. These include (1) evaluating the impact of finite matrix block size on conservative particle transport in fracture networks, and (2) developing a new mesh generation methodology for 3D discrete fracture networks and the adjacent rock matrix.

6.5.2 MODELING THERMAL SLIP OF SINGLE FRACTURES

Background and International Connection: Comparative TM modeling of thermal shear laboratory experiments was conducted under the umbrella of Task G of the DECOVALEX-2023 initiative. The TM subtask of Task G centered on thermal shear as observed in laboratory experiments conducted by KICT. See details on Task G in Section 3.2.2.7 of this report.

Objective: To conduct micro-scale TM modeling of tri-axial laboratory tests focusing on shear processes triggered by thermal stresses.

Associated SFWST Milestone Report: Section 5 in Hu et al. (2024), Crystalline Disposal R&D at LBNL: FY24 Progress, LBNL Report, M4SF-23LB010302033.

Summary:

The Task G sub-task on thermal shearing was motivated by the following key scientific question: Can the shear slip of a stressed fracture be induced by long-term heating effects, and if so, what are the factors that mostly influence the shear slip process? In FY24, LBNL scientists conducted numerical simulations using two different modeling approached - (a) a novel code based on the Numerical Manifold Method (NMM) and (b) the commercial software FLAC3D - for multiscale thermal-mechanical analysis.

In a first step, the two codes were applied to an analytical solution to analyze fracture roughness, strength, shearing and thermal slip at multiple scales. A new model was developed for analyzing the shearing of intersecting fractures and faults—the simplified DFN model—which uses major paths (MPs) to represent complicated DFNs for calculating shearing. To validate the model, LBNL simulated multiple fracture network realizations of various complexity with comparison to MPs using NMM along with a benchmark study on three examples with different simulators applied by different organizations: NMM (LBNL), FLAC3D (LBNL), GBDEM (KIGAM), CASRock (CAS) and FRACOD (DynaFrax). Results from all simulators were compared, showing good agreement with the analytical solution and good consistency between DFN and MP cases.

In a second step, FLAC3D was applied to model the KICT thermal shear experiment. To assess how the asperities affect the thermal slip of single fractures, the LBNL team set up a micro-scale 3D model to explicitly represent the geometry of asperities in two different samples tested by KICT, one with a relatively flat fracture surface, and one with a rough surface. The rough fracture geometry was provided from scanned data of a tensile-split fracture in granite from the KICT experiments that were shared with the DECOVALEX Task G teams. The model was used to investigate the key TM parameters of the host rock and/or the fracture interface and to predict the change in stress in the host rock during thermal shearing. Numerical simulations were compared against the laboratory experiment results of the two granite samples to identify key TM parameters of thermal shearing. A parameter sensitivity study was conducted which suggests that the thermal expansion coefficient and interface configuration (i.e., mated vs. unmated interfaces) have greater impacts on the thermal shearing of single fractures via changing the asperity geometry than simply changing the fracture interface friction angle from 40° to 25° – both resulting in a high effective friction angle if accounting for the geometry of asperities. In addition, it was found that the stress on the asperities of the rough fracture model may have significantly exceeded the typical shear strength of granite minerals (e.g., 70 MPa for quartz), which indicates that the asperities may have failed, which should have significantly impacted the thermal shearing results. These findings were confirmed in comparative evaluation with other Task G modeling teams (see synthesis paper by Kolditz et al., 2024).

6.5.3 MECHANICAL AND HYDROMECHANICAL SIMULATIONS OF A SINGLE FRACTURE

Background and International Connection: The HM subtask of DECOVALEX-2023 Task G centered on experimental data from the GREAT cell (Geo-Reservoir Experimental Analogue Technology) experiments conducted at the University of Edinburgh (McDermott et al., 2018). The GREAT cell is a laboratory experimental setup designed to recreate realistic subsurface conditions exposed to complex multi-directional stress states. See more details on Task G in Section 3.2.2.7 of this report.

Objective: Perform numerical simulations of mechanical and HM processes of a single fracture and compare modeling results against laboratory experiments, focusing on fundamental shear and normal displacement processes under complex 3D stress states.

Associated SFWST Milestone Report: Section 1 in Wang and Hadgu (2024), International Collaboration on Spent Fuel Disposal in Crystalline Rocks, SNL Report, M4SF-24SN010302082.

Summary:

Modeling of mechanical and hydromechanical processes in a single flowing fracture under stress was conducted by SNL scientists using the COMSOL software. Simulation results were compared with experimental data from the GREAT cell, using meshes and stresses for the axisymmetric and triaxial loading cases. Solid mechanics runs were made for stationary (steady state) conditions. Results were analyzed to assess the effects of axisymmetric and triaxial loadings on the surface normal stress, surface displacement, and surface strain. Pressure changes in the fracture between the fluid inlet and outlet were also assessed and used to estimate hydraulic aperture and fracture permeability.

For a purely mechanical case (no fluids involved), an intact uniform resin sample was subjected to axisymmetric and triaxial loading conditions. Model results of circumferential strain closely match the experimental data from the GREAT cell. A hydromechanical modeling case investigated the behavior of existing fractures subjected to coupled hydromechanical processes of shear and normal displacements of the fractures, which could cause material property changes such as permeability. For this modeling case, a cylindrical uniform resin sample with a single vertical fracture was subjected to triaxial loading and fluid flow. For a set of loading positions, pressure changes in the fracture between the fluid inlet and outlet were recorded. The results were used to estimate hydraulic aperture and fracture permeability using the cubic law. Predictions of permeability as a function of normal stress showed a linear negative correlation, which agrees well with the experimental results of Fraser-Harris et al. (2020). These findings were also confirmed in comparative evaluation with other Task G modeling teams (see synthesis paper by Kolditz et al., 2024).

6.5.4 CHARACTERIZING THE IMPACT OF FINITE MATRIX BLOCK SIZE ON PARTICLE TRANSPORT

Background and International Connection: Mass transfer of solutes between fractures and the surrounding rock matrix exerts a noticeable signature on the tail of travel time distributions. The question tackled here is whether the transport characteristics through a discrete fracture network might be affected by the size of the adjacent matrix blocks (finite vs infinite blocks). This activity is loosely connected to Task 10 of the SKB GWFTS Task Force. More details on Task 10 are given in Section 3.4.2.1 of this report.

Associated SFWST Milestone Report: Section 2 in Viswanathan et al. (2024), Crystalline and Crystalline International Disposal Activities, LANL Report, M4SF-24LA010302014.

Objective: To characterize the impact of finite matrix block size on particle transport through fracture networks.

Summary:

Mass transfer of solutes between fractures and the surrounding rock matrix exerts a noticeable signature on the tail of travel time distributions. When the width of the matrix is assumed to be infinite and advective transport through the fracture is sufficiently fast, the tails of the travel time distributions exhibit a classically expected temporal slope. However, studies have yet to characterize how solute transfer between fractures via diffusion through finite matrix blocks influences the tail's slope in three-dimensional fractured media. Thus, in FY24, LANL scientists assessed the impact of finite matrix block size on breakthrough curve (BTC) shape at different spatio-temporal scales by conducting particle tracking simulations in three-dimensional discrete fracture networks. Their study considered a variety of hydrodynamic and geo-structural properties to determine their relative impact on the resulting travel time distributions. It was shown that the travel time distributions through fracture networks with finite blocks are like those with infinite blocks when the fracture spacing is sufficiently large or matrix diffusion is relatively weak. The converse of these conditions results in deviations from the classical scaling. These results provide a first step toward developing a metric to assess when finite block size effects are expected to significantly influence transport, which could be critical for repository assessment.

6.5.5 A NEW MESH GENERATION METHODOLOGY FOR FRACTURE NETWORK MODELING

Background and International Connection: This activity is aimed at developing a new mesh generation methodology for 3D discrete fracture networks and the adjacent rock matrix. The activity is loosely connected to Task 10 of the SKB GWFTS Task Force and Task F of the most recent DECOVALEX-2023. It may also be applied within the “Repository Modeling and Performance Assessment” Task of the current DECOVALEX-2027 phase.

Objective: Develop the near-Maximal Algorithm for Poisson-disk Sampling (nMAPS) to generate point distributions for variable resolution Delaunay triangular and tetrahedral meshes in two and three-dimensions.

Associated SFWST Milestone Report: Section 2 of Hyman (2024), dfnWorks development in support of GDSA, M4SF-24LA01030403, LANL.

Summary:

The near-Maximal Algorithm for Poisson-disk Sampling (nMAPS) was developed by LANL scientists to generate point distributions for variable resolution Delaunay triangular and tetrahedral meshes in two and three-dimensions. The nMAPS provides users with detailed control of the mesh resolution within any region of the domain. Testing of the method showed that it is very efficient, reducing the time for mesh generation in discrete fracture network (DFN) models by two orders of magnitude. A main component of the method is the final meshes that are Delaunay triangular and tetrahedral meshes, which have a dual mesh of a Voronoi tessellation. The corresponding control volumes of the Voronoi tessellations are optimal for flow and transport simulations that use two-point flux finite volume discretization. The use of the *k*-orthogonal and unstructured modeling schemes ensures local mass and volume conservation. The codes FEHM and PFLOTRAN can use these unstructured meshes, which makes them essential for use in complicated geometries that occur within discrete fracture and performance assessment modeling. The nMAPS was integrated into the Los Alamos Gridding Toolkit (LaGriT). Although the method was originally developed for DFN modeling, it has been robustly tested and shown to be useful for a wide range of applications. The algorithm was used, for example, to embedded surfaces into geological formations. This new meshing capability will allow for better representation of geological features and repository structures to be included into GDSA PA simulations.

6.5.6 KEY ACCOMPLISHMENTS

- Task G of the DECOVALEX-2023 project involved TM and HM modeling of single fracture mechanics exposed to complex stress states. Comparison of simulations conducted by national lab scientists with other international modeling teams showed that complex HM and TM experiments results could be well understood and reproduced numerically with sufficient accuracy representing main process characteristics. Micro-scale TM simulations of thermal shearing laboratory experiments identified the key properties impacting shearing behavior in flat and rough fracture surfaces. Modeling results of HM processes evaluated the effects of axisymmetric and triaxial loadings on the surface normal stress, surface displacement, and surface strain, and used these results to estimate hydraulic aperture and fracture permeability changes. The collaborative model comparison conducted in Task G will improve the reliability and predictability of models for fracture flow and transport in crystalline rock.

- Numerical modeling that is loosely related to the SKB GWFTS Task Force focused on characterizing the impact of finite matrix block size on particle transport through fracture networks. It was shown that the travel time distributions through fracture networks with finite blocks are like those with infinite blocks when the fracture spacing is sufficiently large, matrix diffusion is relatively weak, or transport is considered at an early control plane distance. These results provide a first step toward developing a metric to assess when finite block size effects are expected to significantly influence transport, which could be critical for repository assessment.
- A new mesh generation methodology for 3D discrete fracture networks and the adjacent rock matrix (referred to as nMAPS) was developed, robustly tested, and integrated into LANL's powerful gridding toolkit. This new meshing capability will allow for better representation of geological features and repository structures to be included into GDSA PA simulations.

6.6 SALT COUPLED PROCESSES, GEOMECHANICS, AND BRINE MIGRATION

6.6.1 INTRODUCTION

International collaboration has significantly advanced the understanding of complex mechanical, hydrological, thermal, and chemical processes in domal and bedded salt. In FY24, collaborative research with German institutions included bilateral collaborative projects: RANGERS, KOMPASS, and MEASURES. Section 6.6.2 presents a summary of these U.S.-German activities.

SFWST scientists were also involved in international initiatives through the salt-related Task E of the DECOVALEX-2023 initiative and the Salt Club activities under the auspices of the NEA. Section 6.6.3 summarizes Task E of the DECOVALEX-2023, which comprises several modeling steps associated with the BATS test at WIPP. Section 6.6.4 summarizes the NEA Salt Club activities (Mills et al., 2024).

6.6.2 INTERNATIONAL COLLABORATION THROUGH THE RANGERS, KOMPASS, AND MEASURES PROJECTS

<u>Background and International Connection</u>: SFWST scientists and their German colleagues in federal institutions, research laboratories, and academia have a long history of close collaboration on various R&D issues related to the disposal of radionuclide waste in salt. A MoU was signed several years ago between DOE and the German Federal Ministry of Economics and Technology (BMWi) to cooperate in the geologic disposal of radioactive wastes (MoU date: November 2011). The ongoing RANGERS, KOMPASS and MEASURES projects are part of a comprehensive ecosystem of joint salt activities with Germany, which also comprise regular U.S.–German Salt Workshops held to advance collaboration. See more details on salt collaboration with Germany in Section 4.2 of this report with the RANGERS project described in Section 4.1.2.1 and the KOMPASS and MEASURES projects described in Section 4.1.2.2.

<u>Objectives</u>: The RANGERS project aims to develop a guideline for designing and verifying geotechnical barrier systems in repositories in salt formations that incorporates the existing knowledge and experience of BGE, BGE TEC, SNL, and others regarding geotechnical barriers. The KOMPASS and MEASURES projects, collaborations of German, Dutch, American, and British researchers, seek to improve THM models for crushed salt (i.e., run-of-mine or granular salt),

understand crushed salt behavior, and further develop, calibrate, and validate models for crushed salt.

Associated SFWST Milestone Report: Sections 1 and 2 in Mills et al. (2024), Salt International Collaborations FY24 Update, SNL Report, M3SF-23SN010303063.

Summary:

- *RANGERS Project*

  The RANGERS project is finishing its fifth and final year, thus FY24 activities have focused on wrapping up the work (Section 4.1.2.1). SNL scientists continued their State of the Art (SOTA) assessment in science and technology for the design and verification of geotechnical barriers. Eric Simo (BGE TEC) and Kris Kuhlman (SNL) presented three in-person presentations on the RANGERS project at the 14th US/German Workshop in Manchester, UK, titled: (1) RANGERS: Integrity Assessment of a Drift Sealing System, (2) RANGERS: Salt Repository Evolution at Multiple Scales, and (3) RANGERS: Contribution to Process Understanding of Gas Transport in Salt.

  Overall, the RANGERS project has been a worthwhile collaboration on the design, optimization, and modeling of the engineered aspects of repositories for radioactive waste disposal in salt. Bringing together BGE TEC expertise on mechanical modeling and SNL's expertise on flow modeling over the last five years, the collaboration improved our understanding of the problem, and developed key collaborations that will continue in future collaborative efforts (e.g., EURAD-2).

- *KOMPASS and MEASURES Projects*

  The KOMPASS and MEASURES projects are collaborations of German, Dutch, American, and British researchers seeking to improve thermo-hydro-mechanical models for crushed salt (i.e., run-of-mine or granular salt) to be used as backfill for emplacement tunnels (Section 4.1.2.2). KOMPASS ended recently and in FY24 the former KOMPASS partners developed a continuation proposal referred to as MEASURES. Once the MEASURES proposal is approved, funding is expected to begin in late 2024. As part of the MEASURES proposal, SNL began developing a new crushed salt constitutive model to supersede the Callahan model (Callahan, 1999). This new constitutive model will include the following improvements (Coulibaly, 2023): (1) A generalized grain geometry allowing for a consistent transition from porous to intact salt without consideration of ad hoc effective stress and porosity modifications, (2) An anisotropic formulation capable of capturing deformation history, and (3) An application of a physicochemical model as an alternative to the phenomenological approach.

6.6.3 MODELING OF THE BRINE AVAILABILITY TEST IN SALT

Background and International Connection: Comparative THM analysis and modeling of the Brine Availability Test in Salt (BATS) was conducted by a joint team of LBNL, SNL, and LANL scientists according to Task E of the DECOVALEX-2023 project. The objective of Task E was to observe and predict the coupled processes governing the availability of water to heated excavations in geologic salt. Brine availability strongly impacts the long-term performance of salt repositories for heat-generating radioactive waste. See more details on Task E in Section 3.2.2.5 of this report.

Objective: To perform collaborative modeling of the BATS field test at WIPP and to compare simulated and measured responses of brine migration and other THM measurements.

Associated SFWST Milestone Reports: (a) Section 5 in Rutqvist et al. (2024b), Salt Coupled THMC Processes Research Activities, LBNL Report, M3SF-23LB010303032, (b) Section 3 in Mills et al. (2024), Salt International Collaborations FY24 Update, SNL Report, M3SF-23SN010303063, and (c)

Section 2 in Guiltinan et al. (2023), LANL Contributions to Salt International Activities: 2023, Milestone M3SF-23LA010303023. (Note: because the Guiltinan et al. (2023) report summarizing LANL research for FY23 was issued in November 2023, after the deadline of the M2 International Report for FY23, it was not cited in the FY23 International report.)

Summary:

In FY24, LBNL, SNL, and LANL scientists continued analyzing and modeling the BATS coupled salt processes at WIPP, in collaboration with international scientists from Germany, the Netherlands, and the United Kingdom under the umbrella of DECOVALEX-2023 Task E (Section 3.2.2.5). This task ended recently. Thus, the SFWST modeling teams were focused on finalizing the Task E work, wrapping up the final modeling steps, and publishing relevant findings from the comparative modeling activities (e.g., Tounsi et al., 2024). A comprehensive synthesis of the collaborative modeling results is provided in the paper by Kuhlman et al. (2024a), which was co-authored by representatives of all institutions participating in this study. Key modeling results included the cooling-induced increase in brine inflow after heater turn-off and the evolution of damage in rock salt during heating and cooling. Predictions also showed that in the longer term (tens to hundreds of years), it is expected the drift and the damage of the EDZ will creep shut, and the dynamic processes observed in BATS will be less critical.

The participating teams used a broad portfolio of modeling tools: OpenGeoSys (BGR, Germany), COMSOL (COVRA, Netherlands), CODE_BRIGHT (GRS, Germany), QPAC (Quintessa/NWS, UK), FEHM (SNL), TOUGH-FLAC (LBNL) and PFLOTRAN (LANL). There were also a range of approaches from the teams, from mechanistic to prescriptive. Given the uncertainties in the problem, some teams used one- or two-dimensional models of the processes, while other teams included more geometrical complexity in three-dimensional models. Despite these differences, the collective modeling of brine inflow processes led to an increased understanding of the complex processes expected to occur in the EDZ of a salt repository for disposal of heat-generating radioactive waste (Kuhlman et al., 2024a).

Most of the teams participating in Task E of DECOVALEX-2023 are continuing to work together as part of the new BATS2 task in the current DECOVALEX-2027 phase. Like BATS, the BATS2 task centers on a series of borehole heater tests and gas tracer injection tests that were conducted in horizontal boreholes in the EDZ surrounding a drift at WIPP. BATS2 testing is done in the same WIPP tunnel but at a different location. Also, the design of the BATS2 heater array is different from the BATS array, considering lessons learned from the previous experiment.

6.6.4 INTERNATIONAL COLLABORATIONS THROUGH NEA SALT CLUB

Background and International Connection: SFWST scientists and their international collaborators continued progress on a comprehensive FEPs catalog and FEP database for salt repositories. This work was extended through the development of a generalized approach to scenario development for a high-level waste repository at a generic salt site. The latter was done by a Salt Scenarios working group within the NEA Salt Club, bringing together researchers from the US, Germany, Netherlands, and the UK.

Objective: To develop a generalized approach to scenario development for a high-level waste repository at a generic salt repository, with focus on regulations and practices associated with human intrusion scenarios.

Associated SFWST Milestone Report: Section 5 of Mills et al. (2024), Salt International Collaborations FY24 Update, SNL Report, M3SF-24SN010303063.

Summary:

The Salt Scenarios working group continued preparing an NEA Salt Club report on the scenario development, and a journal article was completed (Kuhlman et al., 2024b). The work status was discussed at the in-person NEA Salt Club meeting and the US/German Workshop on Salt Repository Research, Design & Operation in Manchester, UK, in June 2024. This collaborative effort brought together experts on FEPs and scenario development from Germany, the UK, Sandia, and the Netherlands. Preparation of the journal article revealed the similarities and differences in the different programs, often due to regulatory differences. Understanding these differences is essential when transferring lessons learned through experience in international programs to the U.S. disposal program.

6.6.5 KEY ACCOMPLISHMENTS

- Collaborative research with German institutions included (1) assessing geotechnical barriers in salt in the collaborative project RANGERS and (2) improving THM modeling for crushed salt (used as backfill for repository tunnels) in the joint KOMPASS and MEASURES projects.
  - The RANGERS Project completed a comprehensive compilation of existing knowledge and experience about geotechnical barriers in a salt repository. A key outcome of the work is a set of recommendations for designing and verifying geotechnical barriers based on the state of the art in science and technology.
  - The KOMPASS Project completed experimental investigations of microstructural effects on compaction methods and conducted a comparative THM model evaluation. Each modeling partner calibrated their model against laboratory tests performed on KOMPASS reference material, developed model improvements as necessary, and used the resulting calibrated model(s) to simulate the closure of a drift backfilled with crushed salt. As part of the MEASURES proposal, Sandia began developing a new crushed salt constitutive model.
- International collaboration within the framework of Task E of the international DECOVALEX-2023 project allowed SFWST scientists to benefit from the engagement of international partners in the analysis and modeling of brine migration in heated salt. THM modeling conducted by the joint team of LBNL, SNL, and LANL researchers captured the main characteristics observed in the BATS heater experiment at WIPP, including modeling of the cooling-induced increase in brine inflow after heater turn-off and the evolution of damage in rock salt during heating and cooling. This work helped improve understanding of the complex processes expected to occur in the EDZ of a salt repository for disposal of heat-generating radioactive waste and supports building the long-term repository safety case for radioactive waste disposal in salt.
- Under the umbrella of the NEA Salt Club, SFWST and international colleagues continued to develop a comprehensive FEPs database for salt host rock. They extended these efforts towards a generalized approach to scenario development for a high-level waste repository at a generic salt site.

6.7 HYDROMECHANICAL BEHAVIOR OF FAULTS IN RESPONSE TO REPOSITORY-INDUCED PERTURBATION IN ARGILLITE ROCK

6.7.1 INTRODUCTION

Repository-induced effects such as the creation of an EDZ, gas generation, and thermally induced pore pressure perturbations may result in the reactivation of pre-existing fractures, faults, or bedding planes within the host rock, which in turn may cause the formation of permeable transport pathways through the otherwise low-permeability host rock. Understanding such reactivation and its short- to long-term effects is critical in assessing the performance of radioactive waste repositories in clay formations. This section summarizes international collaboration activities where SFWST scientists monitor and simulate the hydromechanical behavior of argillite host rock affected by pore pressure perturbations. These activities are related to a series of highly instrumented controlled-injection fault activation experiments at the Mont Terri URL in Switzerland (Section 3.1.3).

Section 6.7.2 summarizes FY24 work on the data interpretation and modeling of the Mont Terri fault activation experiments, with a focus on long-term sealing mechanisms. Section 6.7.3 highlights the development and application of Machine Learning approaches to analyze the time series data of pore pressure and fault displacements in response to fluid injection into the main fault at Mont Terri.

Note that to date, the fault reactivation experiments at Mont Terri have involved injection at ambient temperature. However, LBNL researchers started planning a controlled thermal stimulation of the fault by deploying 3 m long heaters in boreholes drilled a few meters from the fault zone, at about 40 m depth below the Mont Terri galleries. The objective is to explore whether the heat emanating from decaying waste might create thermal stresses high enough to reactivate a fault. A feasibility test is scheduled for late 2024. Results from this feasibility test will guide the design and execution of a dedicated thermal fault activation test to be conducted in FY25.

6.7.2 SELF-SEALING OF ACTIVATED FAULTS IN ARGILLITE HOST ROCK

Background and International Connection: The field and modeling activities related to the fault activation experiments are conducted with multiple international partners involved in the Mont Terri Project. These partners provide financial and intellectual contributions to the experiment. See more details on the fault activation experiments in Section 3.1.3 of this report.

Objective: Use field observations to evaluate the long-term self-sealing processes of activated faults in argillite host rock at the Mont Terri URL.

Associated SFWST Milestone Report: Section 8 in Rutqvist et al. (2024a), Investigation of Coupled Processes in Argillite Rock: FY24 Progress, LBNL Report, M3SF-24LB010301032.

Summary:

Since 2015, LBNL scientists have conducted a series of fault activation experiments at the Mont Terri URL that highlight the potential for significant permeability increase upon activation and rupture along initially low-permeability faults (Guglielmi et al., 2016; Jeanne et al., 2017; 2018; Cappa et al., 2022). All experiments revealed a rapid increase in fault transmissivity by several orders of magnitude during activation. Subsequent observations conducted after the active injections showed a gradual transmissivity decrease by about three orders of magnitude, with long-term fault creep competing against secondary processes, notably clay mineral swelling. In FY24, LBNL scientists continued their analysis and interpretative modeling of these experiments, with particular focus on the observations and mechanisms that control self-sealing following fault activation. The ability of faults to seal after failure is very important to the long-term performance of clay repositories.

As described in Rutqvist et al. (2024a), the self-sealing assessment focused on the observations made during and after a controlled injection experiment conducted in 2020 in the Mont Terri URL. The intentional activation of the fault caused a significant permeability increase. After the fluid injection was stopped, the post-activation sealing of the fault was monitored for approximately one year. The transient transmissivity recovery of the fault was measured with pulse tests repeated every 2 to 4 weeks. The LBNL team identified several key mechanisms contributing to the observed self-sealing phenomena following the activation of a shale fault:

- Increase in effective normal and shear stress associated with the mechanical closure of the fault under depressurization conditions.
- Steady-state compacting creep occurs within the range of laboratory values, considering the same state of stresses and similar argillaceous rock types.
- Very long-term fault expansion: this may be linked to the swelling of clay minerals.

These mechanisms dominate the self-sealing process over distinct time scales. Initially, a fast response to depressurization operates over a few days, followed by steady-state creep over months, and eventually, swelling over years. Different fault transmissivity versus time relationships were developed to characterize the data and predict sealing delay times for clay-rich fault zones. Due to the multiple competing processes involved, describing the fault sealing process with a single relationship proved challenging. All conceptual models employed to interpret the field data converge on estimating that the fault's return to its initial low transmissivity state would require a minimum of 50 years. This finding holds significance in the context of radioactive waste repositories in clay host rock.

6.7.3 MODELING INJECTION-INDUCED FAULT SLIP USING LONG SHORT-TERM MEMORY NETWORKS

Background and International Connection: ML approaches provide an alternative yet powerful modeling framework that can address some of the limitations of physics-based numerical modeling. By learning from sufficient data, ML can predict physical changes in time and space without explicitly solving complex coupled physical processes such as fault reactivation. In this FY24 activity, Machine Learning is used to analyze the time series data of pore pressure and fault displacements in response to fluid injection into the main fault at Mont Terri. See more details on the fault activation experiments in Section 3.1.3 of this report.

Objective: To develop a ML model that can predict the evolution of pore pressure and fault displacements in response to fluid injection based on the Mont Terri fault slip experiment.

Associated SFWST Milestone Report: Section 6 of Rutqvist et al. (2024a), Investigation of Coupled Processes in Argillite Rock: FY24 Progress, LBNL Report, M3SF-24LB010301032.

Summary:

This study investigated applying a Long Short-Term Memory (LSTM) based ML model to predict fault displacement and pore pressure in response to the 2020 injection into the Main Fault at Mont Terri (see Section 6.7.2). The experiment involved controlled fault activation using six injection cycles. This study focused on modeling the fault response near the injection borehole. A specific protocol using a recursive approach was developed for training the ML model: To model pore pressure and fault displacements (at a given time step, injection at the current time step and the previous n – 1 time step is considered. In addition, pore pressure and displacements from the previous n time steps are considered. Five numerical experiments were conducted, each comprising a different combination of injection cycles used for training and testing, to investigate the ability of the developed ML model to predict fault pressure and displacements.

Simulations showed that the LSTM based ML model could capture pressure and displacement peaks accompanying an increase in fluid injection and the decay in pressure and displacement during the injection shut-in period. The model's predictive ability, however, is highly dependent on the physical processes of fault behavior observed during the training process. For example, if the fault response in a training data set does not capture the highly irreversible dilative fault slip response experienced in another data set, the ML model is unable to reproduce such behavior. The ML model would need to be improved to simulate the dilative behavior of the fault adequately.

6.7.4 KEY ACCOMPLISHMENTS

- SFWST scientists advanced the data and modeling analysis of the Mont Terri fault reactivation experiments to explore the ability of reactivated faults to self-seal over time. The integration of *in-situ* experiments and modeling revealed several key mechanisms contributing to the observed self-sealing phenomena following the activation of a shale fault. Time estimates for the return of a fault to its initial small transmissivity project a minimum of 50 years.
- An efficient ML approach was developed for simulating the fault reactivation process based on data from the 2020 fault reactivation conducted at Mont Terri. LBNL researchers tested a specific protocol for training the ML model, which ensures that the model can accurately represent the complex fault response both qualitatively and quantitatively during and after injection.

6.8 FIELD-SCALE CHARACTERIZATION OF FRACTURES IN CRYSTALLINE ROCK

6.8.1 INTRODUCTION

Since 2015, LBNL has been cooperating with the COSC scientific deep-drilling project in Sweden (see more details in Section 4.3). Investigations have been conducted using the COSC-1 borehole as a testbed for improved site characterization techniques of crystalline repository systems, especially to characterize fractures and their hydrogeologic properties. In 2020 and 2021, LBNL scientists deployed a novel downhole probe (referred to as SIMFIP) in the COSC-1 borehole to identify flowing fractures, evaluate their HM properties, and estimate the state of stress in the subsurface. Continued analysis of the monitoring and testing results from COSC-1, specifically to understand how the 3D displacements may affect the state of stress in the deep subsurface, is described in Section 6.8.2. This work led to the development of a multi-step monitoring workflow for the *in-situ* characterization of fractures including their hydromechanical properties and stress states. The workflow was independently tested to characterize a fractured fault zone in granitic rock at 1 km depth in the Bedretto URL situated in the Swiss Alps.

6.8.2 USING 3D DISPLACEMENT MEASUREMENTS TO DETERMINE STRESS STATE AND STRESS HETEROGENEITY

Background and International Connection: This activity involves collaboration with the international COSC scientific deep drilling project in Central Sweden. Being able to use the COSC-1 borehole provided a valuable opportunity to test field characterization techniques for crystalline host rocks. See more details on COSC in Section 4.3 of this report. Further testing of the SIMFIP probe for characterization of a fractured fault zone in granitic rock was conducted at the Bedretto URL in Switzerland (see Section 4.4), which is accessed from a 5 km long tunnel under the Swiss Alps with an average overburden of ~1 km of crystalline rock.

Objective: (a) To develop a new *in-situ* workflow to characterize stress tensor variations and fracture hydromechanical (HM) properties at large depths of 500 m to 1 km in the COSC-1 borehole, and (b) to independently test the new workflow to measure the flow and mechanical properties of a fractured fault zone in crystalline rock at the Bedretto URL in Switzerland.

Associated SFWST Milestone Report: Section 3 in Hu et al. (2024), Crystalline Disposal R&D at LBNL: FY24 Progress, LBNL Report, M4SF-24LB010302033.

Summary:

In FY24, LBNL scientists continued to analyze the results of water flow measurements, pressure, and displacements from the COSC-1 borehole to evaluate the flow and mechanical properties of crystalline rock at large depths from 500 m to 1 km, including borehole sections that were unfractured or fractured with both sealed and flowing fractures. The Step-rate Injection Method for Fracture *In-situ* Properties (SIMFIP) tool was upgraded to perform measurements at considerable depths under elevated pressure. The multi-step workflow for *in-situ* characterization of fractures using SIMFIP was successfully deployed to characterize a deep rock using a single HQ diameter characterization borehole. The work performed at COSC demonstrated that adding borehole displacements to a hydraulic test allows for an accurate estimation of fracture HM properties (stiffness, hydraulic aperture), intact rock bulk and shear moduli, and local state of stress.

The analysis of experimental data from the COSC-1 borehole showed that intact rock bulk modulus values are consistent with other laboratory-scale estimations for investigated metamorphic rock. Closed fracture stiffness is close to intact rock stiffness, but these fractures can reopen at high pressure, and their stiffness becomes intermediate between natural fractures and intact rock. It was found that naturally flowing fractures appear to display the lowest stiffness values, and a simple hydraulic aperture variation with the fracture's normal displacement reasonably matches the measurements. Displacement measurements showed the strong influence of borehole wall deformation on the onset of fracture activation. After several fracture reopening cycles, this influence vanishes, and hydromechanical movements of the fractures mainly drive displacements. Thus, the borehole wall displacement can be used to estimate intact rock and fracture properties such as the bulk and shear moduli and the fracture normal and shear stiffness. The results indicate that a mechanical weakening phase precedes flow into the deeper host rock, i.e., several stimulation cycles are needed to trigger flow through the borehole damage zone.

To demonstrate that the SIMFIP deep borehole characterization workflow is mature, the LBNL team recently deployed the probe to estimate stresses in a faulted granite in the Bedretto URL (Switzerland), which provides straightforward access to a natural Alpine fault zone at a 1 km depth. This first Bedretto tests highlighted how a fault zone can create much more significant stress perturbations compared to single fractures (as observed in the COSC-1 experiments in Sweden). It was also found that the fault properties favor fault activation and eventual permeability change at fluid pressures lower than the Coulomb stress. More experimental and interpretative work related to the Bedretto URL will be conducted in FY25.

6.8.3 KEY ACCOMPLISHMENTS

- In cooperation with the COSC deep drilling project in Sweden, the deep borehole COSC-1 was used as a testbed for advanced site characterization of fractured crystalline rock. SFWST scientists developed and tested a new workflow using novel downhole probes to identify flowing fractures, evaluate their HM properties, and estimate the state of stress in the subsurface.
- Analysis of the COSC-1 data demonstrated that adding borehole displacement measurements to a standard hydraulic fracturing test allows for an accurate estimation of fracture HM properties (stiffness, hydraulic aperture), intact rock bulk and shear moduli, and local state of stress.
- Compared to the COSC-1 experiments in Sweden, the field test conducted in a faulted granite in the Bedretto URL (Switzerland) highlighted that a fault zone creates significantly greater stress perturbations than single fractures.

6.9 PERFORMANCE ASSESSMENT AND RADIONUCLIDE TRANSPORT MODELING

6.9.1 INTRODUCTION

SFWST researchers have collaborated with international colleagues on building confidence in modeling and software development for the PA of deep geologic repositories. Task F of the

DECOVALEX-2023 involved comparison of PA modeling results from multiple international modeling teams, applied to the same reference cases, to enhance confidence in PA modeling (Section 3.2.2.6). The teams developed PA modelling skills and capabilities, analyzed the influence of model choices and parameters on the assessment of repository performance, and compared the uncertainties introduced by model choices to other sources of uncertainty. Because Task F involved no actual experiment or site, the PA modeling exercise required the conceptual development of two hypothetical repository designs and geologic settings that were conducted in parallel: a repository for commercial spent nuclear fuel (SNF) in a fractured crystalline host rock (with nine participating modeling groups), and a repository for commercial SNF in a bedded salt formation (with four participating modeling groups). The foundational aspects of this study, such as methods of coupling process models, propagating uncertainty, and conducting sensitivity analysis, are expected to be transferable between the two reference cases. The GDSA team at SNL led this task, which has now ended. However, the comparison of performance assessment approaches continues in the current DECOVALEX-2027 phase (see Section 3.2.3.8), with an enhanced focus on sensitivity analysis and uncertainty quantification. Subsection 6.9.2 summarizes FY24 research activities related to Task F of DECOVALEX-2023.

Developing and implementing adequate thermodynamic and thermochemical databases and models across broad physicochemical conditions is essential for understanding, evaluating, and modeling geochemical processes, such as speciation, solubility, and reaction paths. SFWST researchers at LLNL are collaborating with international colleagues to improve the thermodynamic and thermochemical databases and models needed to evaluate radionuclide transport through the EBS materials and host rock. These studies are intended to provide updated datasets for modeling the reactive transport of radionuclides, a central component of PA models, as they evaluate transport from the repository to the biosphere for dose calculations. Section 6.9.3 summarizes the FY24 development of these databases.

6.9.2 COMPARATIVE PERFORMANCE ASSESSMENT MODELING OF CRYSTALLINE AND SALT REFERENCE CASES

Background and International Connection: Confidence in performance assessment predictions can be enhanced by comparing PA modeling results from multiple international disposal programs applied to the same reference cases. Comparative PA modeling of two reference cases was conducted under the umbrella of Task F of the DECOVALEX-2023 Initiative. More details on Task F can be found in Section 3.2.2.6 of this report.

Objective: To build confidence in the models, methods, and software used for the performance assessment of deep geologic repositories, and/or to bring additional research and development needed to improve PA methodologies for generic crystalline rock and salt repositories.

Associated SFWST Milestone Reports: (a) Sections 2 and 3 in Mariner et al. (2024b), DECOVALEX-2023 Task F1 Final Report, SNL Report, M3SF-24SN010304083, (b) Section 3 in Mills et al. (2024), Salt International Collaborations FY24 Update, SNL Report, M3SF-23SN010303063, and (c) Sections 2-5 in LaForce et al. (2024), DECOVALEX-2023 Task F2 Salt Final Report, SNL Report, M3SF-24SN010304093.

Summary:

DECOVALEX Task F aimed at a comparison of the models and methods used in deep geologic repository performance assessment. SFWST scientists have a dual role in Task F: Paul Mariner served as the task lead for the crystalline case (F1) and Tara LaForce had this role for the salt case (F2). In addition, scientists from the SNL GDSA team contributed their own PA modeling for the two reference cases and have compared their results with other international teams.

- *Crystalline Reference Scenario (F1)*

  In previous years, Task F1 prepared for the full repository PA modeling with a set of simplified benchmarks involving flow and transport in fractured rock. The benchmark cases provided an opportunity to understand differences in model implementation that affect how a problem can be specified, what results can be obtained, and the influence modeling choices have on calculated values of performance measures in relatively simple systems.

  In FY24, the eight modeling teams involved in Task F1 finalized PA simulations for a mined repository at a depth of 450 m in fractured crystalline rock. The repository has 50 parallel backfilled drifts, each with 50 deposition holes six m apart. Each deposition hole contains a 4-PWR waste package and bentonite buffer. The rock domain is five km in length, two km in width, and one km in depth. It has six deterministic fractured deformation zones and a multitude of stochastic fractures. Teams generally used the ECPM approach for the entire rock or a hybrid approach in which the deterministic fracture zones are modeled with a DFN and the rest of the rock is modeled by ECPM. Out of eight teams, seven modeled most or all major features and processes of the reference case. The teams developed new modeling capabilities and skills, including upscaling DFNs to an ECPM, new comparison and verification methods, and new ways to model matrix diffusion. In some cases, individual teams developed two or three models to simulate the benchmark cases or tried different resolution meshes. For example, compared to the DFN model, breakthrough tended to be smoother with the ECPM, as expected. The effects of model choices between teams are less clear because of multiple differences in model choices between teams (e.g., gridding, representation of repository features, etc.). Comparison of the results of all models clarify the effects of explicit inclusion of drifts, buffer, and backfill in the reference case models and motivate improved methods to account for the effects of those features. In addition to above listed milestone reports, results from Task F1 are described in two synthesis papers by Mariner et al. (2024a) and Leone et al. (2024).

- *Salt Reference Scenario (F2)*

  Task F2 involved comparison of models and methods for a simplified post-closure performance assessment model of a deep geologic repository in domal salt host rock over 100,000 years. Simulations were conducted assuming a disturbed scenario in which shaft seals fail 1,000 years after repository closure, allowing an influx of brine down the shafts and into the repository. The participating teams conducted modeling using thermal, hydrological, mechanical, and chemical properties of individual components of the engineered and natural systems. Together, the teams used a ground portfolio of modeling approaches, assumptions, and quantities, model dimensionality, filling in the repository, solubility limits, coupling salt compaction behavior, timing of shaft failure, heterogeneous shaft fill, geosphere brine inflow, multiphase flow variants, and changing initial water saturation of the repository, which are explained in detail in La Force et al. (2024). These individual model choices had impact on the PA model responses: for example, teams incorporating creep closure saw increased liquid saturation early in the simulation compared to teams that did not.

  The participating teams applied various model assumptions from compartmentalized networks to full 3D models of the salt formation. However, no single model included a full-fidelity representation of all the FEPs detailed in the task specification. Despite differences in the modelling strategies developed by participating teams (see Table 4-1 to Table 4-5 of LaForce, 2024), all models indicate that salt compaction and radionuclide diffusion are key physical processes in the simplified repository system. Similarly, all models showed that the engineered barriers are effective for containing the radionuclides in the repository and that only a small amount of the disposed radionuclides will migrate beyond the repository seal over 100,000 years.

6.9.3 THERMODYNAMIC AND THERMOCHEMICAL DATABASE DEVELOPMENT

Background and International Connection: Thermodynamic and thermochemical data are essential for understanding, evaluating, and modeling geochemical processes and radionuclide transport. The LLNL activities are aligned with the NEA Thermochemical Database (TBD) Project and include collaborations with the Helmholtz Zentrum Dresden Rossendorf (HZDR, Germany), the Paul Scherrer Institute (PSI, Switzerland), as well as the Karlsruhe Institute of Technology (KIT, Germany).

Objectives: To ensure that PA modeling efforts in the U.S. utilize internationally accepted practices for repository PA calculations and thermodynamic and thermochemical databases, and to develop open-source databases that can be shared and integrated with multiple nuclear waste programs internationally.

Associated SFWST Milestone Report: (a) Sections 2,3, and 5 in Zavarin et al. (2024a), Surface Complexation/Ion Exchange Data Integration for Radionuclide Sorption to Clay Minerals, LLNL Report, M3SF-24LL010301062, and (b) Sections 2-5 in Zavarin et al. (2024b), NEA-TDB Management and International Collaborations in Sorption and Thermodynamic Modeling: Crystalline International Collaborations, LLNL Report, M3SF-24LL010302062.

Summary:

A continuing focus in FY24 has been the improvement of surface complexation and ion exchange data for radionuclide sorption to clay minerals as well as the interacting with the international NEA Thermodynamic Database Project, see details below.

- Surface Complexation and Ion Exchange Database Development

  In FY24, research effort at LLNL was placed on the extension of the surface complexation and ion exchange database (L-SCIE) with focus on clay minerals (predominantly smectite) typical for bentonite and argillite rock. LLNL incorporated the Paul Scherrer Institute (PSI) digitized clay sorption data into the L-SCIE database, which increased the number of references to 267, the datasets to 2667, and individual data points to 33,115. Most of the new data were associated with radionuclide sorption to clay minerals. A summary of the data available in the L-SCIE database is plotted in Figure 1 of Zavarin et al. (2024a).

  The database is also supplemented by sorption references contained in the RES3T database (Helmholtz-Zentrum Dresden-Rossendorf, 2022) and the data captured from the JAEA K_d database. LLNL began developing high throughput automated workflows to model surface complexation and ion exchange of radionuclides on clay minerals focusing on montmorillonite and illite. This approach will be compared to a recent PSI database update (based on non-electrostatic surface complexation) as part of the Swiss repository performance assessment model. The data science-based workflows will provide a major incentive for other institutions to adopt FAIR-formatted, interoperable databases), the PHREEQC geochemical modeling code has been replaced with CrunchFlow reactive transport code (Steefel, 2009). It is planned to replace the PEST parameter estimation tool with Python-based optimization routines to further improve the modeling workflow.

- *Thermochemical Database Development Related NEA Thermochemical Database Project*

  The thermochemical database activity at LLNL focuses on long-term commitment to engaging the partners involved in the international nuclear waste repository research. This includes participation in the NEA-TDB Project and development of methodologies for integrating US and international thermodynamic databases for use in SFWST GDSA efforts. In FY24, a continuing focus was to support the US participation in the NEA-TDB effort, the development of an agreement for a Phase 7 activity that will start in Q1 of 2025.

In FY24, LLNL facilitated the integration of NEA-TDB thermochemical data with LLNL's SUPCRTNE thermodynamic database that supports the SFWST GDSA activities. This effort is coordinated with the Argillite work package SUPCRTNE database development efforts (Wolery, 2024). The goal is to provide a downloadable database that will be hosted on LLNL's thermodynamics website which incorporates NEA-TDB data into the LLNL database where appropriate.

Recently, LLNL also began engagement with the EURAD-2 program initiated by the Karlsruhe Institute of Technology (KIT), Germany. The primary focus of this collaboration is the DITUSC (Development and Improvement of Thermodynamic Understanding for use in Nuclear Waste Disposal Safety Case) project. The DITUSC project is focused on the consolidation and improvement of knowledge to predict processes over long timescales in key fields for geological disposal of radioactive waste. As a "strategic study" within the EURAD-2 framework, this project aims to develop a white paper summarizing the current thermodynamic understanding and promoting new scientific strategies to further support/improve the use of thermodynamics in the Safety Case of nuclear waste disposal facilities. The DITUSC kickoff meeting and an open workshop are scheduled for November 13- 15, 2024, to be held in Barcelona, Spain.

6.9.4 KEY ACCOMPLISHMENTS

- In Task F of the DECOVALEX-2023 project, confidence in performance assessment models and methods was enhanced by comparing PA modeling results from ten international disposal programs applied to the same reference cases, one involving a repository in a fractured crystalline host rock and another featuring a repository in a bedded salt formation.
  - The crystalline reference case highlighted the importance of explicitly including drifts, buffer, and backfill in the simulations. For models with a comparable repository geometry and inventory evolution, the main source of model uncertainty was in the choices of how to represent the fracture network and simulate transport of two tracers. Overall, the modeling results show considerable differences and demonstrate the importance of examining multiple modeling approaches in performance assessment.
  - Despite differences in the modelling strategies, all PA models for the salt reference case showed that the engineered barriers are effective for containing the radionuclides in the repository and that only a small amount of the disposed radionuclides will migrate beyond the repository seal over 100,000 years. All models also indicate that salt compaction and radionuclide diffusion are key physical processes in the simplified repository system.
- SFWST scientists play a key role in disseminating sorption data and acting as good data stewards by updating the database in a consistent format and assessing the quality of the newly assimilated data in an organized fashion. To this end, all data and workflows are open access and made available on this website: https://seaborg.llnl.gov/resources/geochemical-databases-modeling-codes.
- Continued international collaboration of LLNL researchers within the NEA Thermochemical Database Project led to significant improvement in thermodynamic and thermochemical databases and models for radionuclide transport simulations. The goal is to produce interoperable open-source databases that harness modern data science workflows and algorithms.

6.10 DEVELOPING A DIVERSE NEXT GENERATION WORKFORCE FOR RADIOACTIVE WASTE DISPOSAL

6.10.1 INTRODUCTION

Investing in the next generation of diverse, talented nuclear waste scientists and leaders is vital to fulfilling DOE NE's mission of developing solutions for the long-term geologic disposal of radioactive waste. In FY22, SFWST established a three-year Next Generation Workforce Development Pilot Program to attract, train and advance a talented and diverse future workforce in disposal research. LBNL and SNL started the program in FY22, and LANL was brought into the program in FY23. While FY24 marks the final year of the three-year pilot, the program has been a great success and SFWST envisions continuation of the program into the foreseeable future. International collaboration is important in this context: To help recruit and train a broad talent pool, the workforce development program provides interesting learning/research challenges and attractive work-abroad opportunities in conjunction with SFWST's multiple international collaboration partners. This section summarizes the program activities from FY22 to FY24.

6.10.2 OVERVIEW OF WORKFORCE DEVELOPMENT ACTIVITIES AT LBNL, SNL AND LANL

<u>Background and International Connection</u>: International training programs and international research activities provide valuable opportunities for attracting and training talented young scientists. To tap into these opportunities, SFWST in FY22 established a three-year Next Generation Workforce Development Pilot Program to attract, train and advance a talented and diverse future workforce in disposal research.

<u>Objectives</u>: From FY22 to FY24, the pilot program activities at LBNL, SNL, and LANL focused on the following objectives:

- Stimulating Student Interest in Nuclear Waste Research: This involves coordinating seminars and summer classes, working with minority serving universities, establishing a virtual seminar series for interested undergraduate/graduate students and young nuclear waste disposal researchers, and organizing student participation in existing international training programs.
- Creating the Pipeline: Through undergraduate and graduate internship programs, provide internship opportunities with students from minority-serving institutions placed into selected disposal research activities. Intern projects may be related to international research activities conducted at national labs and may include opportunities to spend some research time at an international partner institution.
- Advancing the Pipeline: Developing postdoctoral research opportunities, which includes providing for one dedicated postdoc position at each institution in a research project with international collaboration while specifically recruiting at minority-serving institutions. Postdoc research projects include opportunities to spend some research time at international partner institutions.

<u>Associated SFWST Milestone Reports</u>: (a) Zheng et al. (2023b), Developing a Diverse Next Generation Workforce for Radioactive Waste Disposal: LBNL Activities in FY23, LBNL Report, M3SF-23LB010307042, (b) Mendez (2024), Developing a Diverse Next Generation Workforce for Radioactive Waste Disposal: SNL Activities in FY24, SNL Report, M4SF-24SN010307052, and (c) Mantelli et al. (2024), Workforce Development LANL 2024, LANL Report, M4SF-23LA010307031, LA-UR-24-28816.

<u>Summary</u>:

- *LBNL Activities*

  A webinar series "Next Generation Workforce Development for Spent Fuel and Waste Science and Technology" with 7 talks was co-organized by MIT, Texas A&M, SNL, and LBNL. Initiated in January 2024, the seminar has reached a broad audience with an average attendance of around 50-60.

  A summer internship program "INGENUITY" (https://sites.google.com/lbl.gov/eesa-student-opportunities/nextgen-nuclear-waste-disposal-internship), initially launched in FY22, just finalized the hiring of interns for the summer of 2024. Applications came from 38 universities with nationalities of 14 countries. Between 2022 and 2024, a total of 19 summer interns have participated and will participate in research projects at LBNL across a variety of disciplines (geochemistry, geomechanics, and geophysics). After a productive summer internship, all summer interns in the 2022 cohort and three summer interns in the 2023 cohort had continued research work with their mentor without pay, two interns returned for a second summer, and three interns were hired at LBNL as postdoctoral researchers. Research conducted by interns also contributed to scientific publications. For example, Elijah Adeniyi who attended the summer program in 2023 contributed to developing machine learning surrogates for surface complexation models of uranium sorption (Li et al., 2024).

  A postdoctoral researcher, Radhavi Abeysiridara Samarakoon, was hired at the end of FY22 and dedicated all her effort to the HotBENT project, an international collaborative project that studies the evolution of bentonite buffer under high-temperature heating. She successfully developed coupled a thermal, hydrological, and mechanical model for the HotBENT field test and contributed to a related SFWST milestone report (Zheng et al., 2023b) and conferences (e.g., Samarakoon and Zheng., 2024). She also attended two courses at the Grimsel Training Centre in Switzerland: "Data Management - Making Geoscientific Data FAIR" and "*In-situ* Testing and Hydraulic Characterization in URL" (https://www.grimsel.com/grimsel-training-centre-gtc).

- *SNL Activities*

  SNL has been working with multiple universities to develop lectures and seminars to promote research in disposal of high-level waste. For example, SNL collaborated with the University of New Mexico Department of Nuclear Engineering to develop and deliver a lecture series centered around current topics and challenges in radioactive waste management. The lectures started in FY22 and supported the Radioactive Waste Management coursework and culminated with a tour of SNL facilities early in FY24. SNL has also been collaborating with the University of Puerto Rico, Mayaguez, to support the Mechanical Engineering Graduate Seminar. SNL researchers in Radioactive Waste Management developed and delivered a series of virtual talks to introduce students to the field of Radioactive Waste Management and the work performed at the National Labs. SNL is also one of the partners of the webinar series "Next Generation Workforce Development for Spent Fuel and Waste Science and Technology" with seven talks. Sandia furthermore collaborates with Texas A&M on a two-week course titled "Backend of the Nuclear Fuel Cycle and Radioactive Waste Management, Storage and Disposal."

  Over the past three years, several summer interns (graduate and undergraduate) hired through the workforce development program were converted to year-round internships working on Disposal Research work packages. While on this program, two undergraduate interns completed their degree in 2023 and are continuing to participate in workforce development as graduate students. In addition, one graduate intern transitioned to "all but dissertation" status and is making progress to finish the PhD degree in the coming year. They all remain in the workforce development pipeline and have transitioned from Workforce Development funds to directly funded projects. In FY24, Sandia recruited three additional graduate summer interns working on a diversity of projects.

After an extensive search in FY22, Sandia was able to identify and hire a postdoctoral appointee to support the SFWST program during FY23. The successful candidate, Dr. Lisa Bigler, holds a PhD in Mathematics from Oregon State University and came to Sandia with previous internship experiences at both LBNL and ORNL. Dr. Bigler was converted to staff in early FY24 and continues to work with the team in GDSA RSA, incorporating geology into UQ/SA.

- *LANL Activities*

  LANL joined the pilot program in the middle of FY23 and started initiating a student intern program via building a website and promoting the program at meetings and conferences. A post-master's student was hired with the funding allotted in August of 2023. Isaac Mantelli has made great strides in the hydrothermal lab and has become an integral part of all experimental work packages. He also revitalized the wet chemistry lab in this short period of time. He contributed to several of LANL's SFWST milestone reports and attended the national SFWST workshop in Las Vegas NV (July 2024).

6.10.3 KEY ACCOMPLISHMENTS

- Stimulating Student Interest in Nuclear Waste Research: Between FY22 and FY24, the Next Generation Workforce Development Pilot Program inspired many students via lab-university organized lectures and seminars to become interested in nuclear waste disposal science. In-person and hybrid lasses were held at the University of New Mexico and the University of Puerto Rico ~ Mayaguez. A webinar series named "Next Generation Workforce Development for Spent Fuel and Waste Science and Technology", co-organized by MIT, Texas A&M, SNL, and LBNL, was held through FY24.
- Creating the Pipeline: The summer internship program trained a large diverse student group of 29 interns. This clearly created a pipeline: Many of the summer interns returned to their hosting national lab (or other opportunities) after their initial summer program ended, either for another summer program or in some cases as year-round interns. At LBNL, three summer interns were later hired as postdoctoral researchers.
- Advancing the Pipeline: LBNL and SNL each hired a dedicated "next generation" postdoc for a three-year research project with international collaboration, which allowed them to make remarkable research contributions. For example, LBNL's dedicated post-doc works on THM modeling for the international HotBENT Project and, to better connect her with the international community, participated in a 2023 summer training program at the Grimsel Test Site. SNL's dedicated postdoc works in GDSA RSA, incorporating geology into UQ/SA.

7 SUMMARY AND CONCLUDING REMARKS

This report describes the FY24 status of international collaboration focused on investigations of nuclear waste disposal in geological formations as part of the DOE SFWST campaign. Since 2012, the SFWST campaign has actively collaborated with several international geologic disposal programs in Europe, North America, and Asia. The joint research activities with international programs, initiatives, and projects are extremely beneficial to SFWST's disposal research program, because they: (1) provide first-hand access to the decades of experience that our international partners have gained in various disposal options and geologic environments, (2) give SFWST scientists an extensive library of experimental data from many past and ongoing *in-situ* tests conducted in several URLs in different host rocks, (3) provide a framework for active peer-to-peer research participation in international groups that conduct, analyze, and model performance-relevant processes, and (4) open the door to conducting SFWST *in-situ* experiments in international URLs not available in the U.S. Last not least, international collaboration allows the SFWST campaign to benefit from substantial international investments in research facilities (such as underground research laboratory testing and modeling) and achieve cost savings via joint funding of expensive field experiments.

This report provides an in-depth overview of the various opportunities for international collaboration available to SFWST researchers, with a primary focus on those opportunities that involve field experiments in international URLs. Section 3 of this report contains a summary of current and previously active international opportunities resulting from DOE's formal partnership in collaborative initiatives: the Mont Terri Project (since 2012), the DECOVALEX Project (since 2012), the SKB Task Forces (since 2014), and the HotBENT Project (since 2018), as well as in past years the Colloid Formation and Migration Project (2012 – 2015) and the FEBEX Dismantling Project (2015–2018). All of these are multinational initiatives with emphasis on field experiments in international URLs. Other multinational initiatives, such as several NEA-coordinated activities, provide valuable opportunities for information exchange and data assessment. Additional opportunities for multinational collaboration exist: For example, SFWST just instituted a technical partnership with the EURAD-2 European Commission collaborative research program which initiated a new round of repository R&D work for a 5-year period from 2024 through 2029. The SFWST campaign has also explored direct bilateral opportunities for active research collaboration, with institutions from Germany, Republic of Korea, Sweden, Israel, France, Japan, Belgium, Finland, Czech Republic, and China. Some of these opportunities have resulted in close bilateral research activities between SFWST scientists and their international counterparts; the others provide opportunities for active research collaboration in the future.

Over the years, as research priorities have changed and new opportunities for collaboration developed, SFWST's international research portfolio has evolved and will continue to evolve. The SFWST program has made a targeted effort to reassess its international collaboration activities on a regular (annual) basis. Section 5 describes the continued planning process which comprises (1) re-evaluating ongoing international research activities, (2) assessing the technical merit of new collaboration opportunities, and (3) revising the overall portfolio of international R&D activities as appropriate. Given its importance within the overall portfolio of disposal research activities, any such planning and prioritization is done in tight integration with other disposal research areas, e.g., the host-rock-specific, EBS, and performance assessment work packages. Section 5 also gives a brief high-level overview of the major R&D themes and international experiments that SFWST researchers have participated in since 2012, either as active experimental team members or as researchers involved in the interpretative evaluation and modeling of the experimental data.

Section 6 gives summaries of specific FY24 research activities in the SFWST campaign which have been conducted under the umbrella of the international collaboration. A comprehensive list of research activities attests to the fact that SFWST researchers have effectively used these opportunities and international collaboration activities formed a considerable portion of the SFWST campaign's disposal research program. International collaboration is a prominent element of key work packages, such as the EBS, Crystalline, Argillite, and Salt Work Packages, and more recently also in the GDSA Work Packages. Therefore, international collaboration in a balanced portfolio of relevant R&D challenges addresses such essential research areas as engineered barrier integrity, near-field perturbations, radionuclide transport, integrated system behavior, performance assessment, site characterization, and monitoring approaches.

Substantial scientific and technical advances have been made over the past years. The joint R&D with international researchers, the worldwide sharing of knowledge and experience, and the access to data for field and laboratory experiments from a variety of URLs and host rock have helped SFWST researchers significantly improve their understanding of the current technical basis for disposal in a range of potential host-rock environments. SFWST 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. Advanced simulation models have been verified and validated against these experimental data, providing a robust modeling and experimental basis for the prediction of the complex processes defining the performance of a multi-barrier waste repository system. In addition, international scientists have contributed to the analysis and interpretative modeling of laboratory or field studies performed by SFWST, such as the HotBENT Lab Experiment and the BATS field experiment. Comparison of model results with other international modeling groups, using their simulation tools and conceptual understanding, has enhanced confidence in the robustness of predictive models used for performance assessment. In addition, the possibility of linking model differences to conceptual model setup has provided valuable guidance into "best" modeling choices and understanding the effect of conceptual model selection on prediction uncertainty. Such advances in the ability to make long-term predictions of complex coupled THMC and flow and transport processes contribute directly to improved post-closure PA models. Access to international field testing has also provided an opportunity to develop, test, and demonstrate new methods and workflows for site characterization and monitoring of deep geological disposal.

In the SFWST campaign, the work packages for international collaboration, EBS, host-rock-specific topics, and performance assessment are well integrated to make optimal use of improved process models leading to better safety assessment models. International collaboration has allowed for the engagement of U.S. researchers with the international waste management R&D community, which helped implement best practices, new science advances, state-of-the-art simulation tools, and lessons learned, and has provided ample opportunity for training/educating junior staff to move a disposal program forward into the next decades.

Below are brief highlights of selected research areas where international collaboration has resulted in significant scientific advances that are relevant not only to SFWST's disposal program but also to the broader radioactive waste management and disposal community.

Progress Related Coupled Processes and Alterations in Bentonite-Based Engineered Barrier Systems (Section 6.1)

Collaborations with the international FEBEX-DP, HotBENT, and Horonobe EBS projects involve large-scale experimental and modeling studies to better understand temperature-dependent perturbations and alterations in engineered barrier materials. These activities have provided valuable insights into how these perturbations and alterations may affect repository performance.

- Participation in the large-scale FEBEX *in-situ* heater test and its comprehensive dismantling effort after 18 years of operation has significantly enhanced the understanding of the thermal alteration of EBS materials. The post-mortem FEBEX-DP bentonite samples continue to provide a basis for evaluating potential EBS property changes. The results of laboratory-scale experiments investigating coupled microbial-abiotic processes in altered and unaltered bentonite samples indicate considerable metabolic potential within the microbial communities even after long-term exposure to heat. This is important because microorganisms that survive in a nuclear waste repository can later become active as gas is introduced or produced in the system, water is introduced through cracks in the containment, or other environmental changes.

- Since reaching its final target temperature of 175°C or 200°C in June of 2022, the HotBENT field test has continued providing data on bentonite behavior at strongly elevated temperatures, which are now used for interpretative modeling. LBNL has developed a 3D TH model which is able to match the trends observed in the thermal and hydrodynamic behavior of the EBS. However, the current model underpredicts the temperature in the bentonite near the heaters. LBNL plans to extend the 3D TH model to a 3D THM and possibly THMC model, which will improve the model predictions, especially when it comes to the buffer's hydration behavior.
- In support of the HotBENT field test, SFWST researchers conducted a series of high-temperature laboratory column tests using innovative geophysical imaging techniques. In FY24, the team studied and simulated results from the HotBENT-Lab #2 column test, which used granulated Wyoming bentonite and lasted for 16 months. The laboratory experiment provides a unique data set of the spatio-temporal change of bentonite properties affected by hydration, heating, and swelling.
- TH simulations were conducted with the PFLOTRAN simulator to understand engineered barrier alterations associated with the JAEA EBS design concept. This work was done under the umbrella of the DECOVALEX-2023 model comparison project, where Task D comprises the full-scale EBS Experiment at the Horonobe URL in Japan. It was shown that a reduced order 2 D model, instead of a full 3 D model, can well represent the general temperature trends. Improvement of the 2-D PFLOTRAN model is needed to simulate fluid flow affected by mechanical processes, such as bentonite swelling and related couplings with porous media flow.

Progress Related to Interfacial Processes Between EBS and Host Rock Materials (Section 6.2)

Several international collaboration studies made important progress in evaluating interfacial reactions between EBS components and host rock materials. Materials alterations in the vicinity of these interfaces can affect repository performance in multiple ways, for example by changing the flow and transport properties for radionuclides to migrate from the engineered into the natural barrier systems. Interfacial reactions are most prominent early in the lifetime of a repository when EBS components such as bentonite backfill, metal containers, and cementitious materials have just been emplaced and when TH perturbations remain strong.

- Hydrothermal laboratory experiments were conducted to better understand interfacial material alterations at conditions relevant to the EBS experiment at the Horonobe URL in Japan and the HotBENT experiment at the Grimsel Test Site in Switzerland. The experimental findings suggest that the tested bentonites may only experience slight alteration during the initial thermal pulse in a repository setting. The mineralogical and geochemical changes observed in both experimental settings can be applied to develop conceptual and numerical models for the assessment of long-term material stability in a high temperature repository.
- Laboratory experiments were conducted to study bentonite erosion, coagulation/flocculation, and fracture clogging behavior under controlled conditions. Results demonstrated the need to develop a new experimental setup to study erosion and coagulation from a single experimental system because a combination of erosion and coagulation will ultimately govern colloid transport. Future experiments will be conducted using unaltered versus hydrothermally aged/altered bentonite to understand the parameters that significantly impact bentonite erosion and coagulation in geochemical conditions relevant to nuclear waste repositories. This work is loosely connected to international collaboration efforts conducted in the CFM and FEBEX projects.

- Reactive transport simulations were performed to interpret interfacial reactions and their impact across aged bentonite, concrete/cement, and clay rock interfaces. These activities were aligned with: (1) the international CI-D experiment, which probes diffusive transport across materials placed in a borehole at the Mont Terri URL about 14 years ago, and (2) the reactive-transport modeling of cement-bentonite interaction as part of the SKB EBS Task Force Task 12 benchmarking activities:
  - Simulations of the CI-D cement-clay interaction test at Mont Terri using the CrunchClay software, which considers electrostatic effects in the EDL models, demonstrated the need to extend the duration of modeling and use a more comprehensive reaction network to predict long-term cement and cement-clay interactions.
  - The Task 12 benchmarking of geochemical changes due to cement-bentonite interaction showed substantial changes in pore solution chemistry, particularly at early times. This can lead to considerable alteration of highly soluble minerals, which in turn can significantly change the porosity and permeability near the interface, possibly impacting the long-term migration of radionuclides through a cement-bentonite EBS. However, the simulations also demonstrated that areas with strong mineral alteration are limited to a few cm next to the interface. Future work should be devoted to evaluating the safety implications of these complex interfacial alterations.

Progress Related to THM Processes in Heated Argillaceous Rock (Section 6.3)

Through access to several *in-situ* heater experiments, SFWST scientists made significant scientific advances in understanding and predicting the THM perturbations occurring in argillaceous host rock after the emplacement of heat-emanating radioactive waste.

- The full-scale FE heater test at Mont Terri, now in its 10th year of heating, continues to provide valuable THM data at relevant spatial and temporal scales. Under the umbrella of Task C of the DECOVALEX-2023 initiative, SFWST researchers and several international partners worked on interpretative and comparative THM simulations for model validation. Based on a comprehensive sensitivity study, the teams were able to achieve an excellent overall match with the measured pore pressure changes in the host rock when considering reduced near-field permeability and increased fluid storage. After completing the work with DECOVALEX-2023, LBNL will resume regular Mont Terri project simulations of the 10-year field data at the FE Experiment. The work for the Mont Terri project will focus on the interaction of the host rock with the bentonite buffer and the stress changes in the bentonite buffer.
- The ability to simulate processes and mechanisms of thermal fracture initiation was tested in Task A of the DECOVALEX-2023 initiative. Modeling of the CRQ *in-situ* heating experiment at the Bure URL showed that different THM modeling approaches were able to reproduce fracture initiation in the COx clay rock in terms of time of occurrence and location whereas attempts to reproduce fracture aperture or fracture propagation were less accurate and require more work in the future.

Progress Related to Gas Transport in Bentonite and Clay-Based Host Rock (Section 6.4)

Gas generation from canister corrosion and other processes can impact the performance of a geological disposal facility in several ways: the gas-water interfaces serve as an important vehicle for the transport of radionuclides and microorganisms due to channelized flow and preferential sorption, whereas trapped gas bubbles can cause accumulation or immobilization of radionuclides. Local pressure build-up due to gas production and accumulation can trigger mechanical responses such as deformation or fracturing in low-permeability materials like bentonite and clays. Significant progress was made in understanding the short- and long-term processes involved in the generation and migration of repository gases.

- Under the umbrella of the DECOVALEX-2023 initiative, SFWST scientists and their international partners tested their predictive capabilities for gas migration against data from the full-scale LASGIT experiment conducted at the Äspö Hard Rock Laboratory in Sweden. LBNL scientists were able to show that an HM modeling approach that was initially developed to simulate small-scale gas injection laboratory experiments could be extended to match the LASGIT field observations.
- A new conceptual model was developed to best capture the complex phenomenological behavior of gas flow through bentonite. The new model can represent observed gas migration patterns such as rapid breakthrough, aperiodic/chaotic gas flux, fast percolation, and low gas saturation. Due to fractal scale invariance, this may provide a new perspective for upscaling from small scale laboratory observations to a field scale. Based on the theory of the linear stability analysis, it was shown that gas channelling can emerge from the morphological instability of the interface between the injected gas and the compacted bentonite due to local stress concentration, pore dilation, and hydrologic gradient variation.

Progress Related to Coupled Processes, Fluid Flow, and Transport in Fractured Crystalline Rock (Section 6.5)

Because crystalline formations are often fractured, repository performance assessment studies require an understanding of (1) the impact of stress changes and other perturbations on fracture flow and transport properties, and (2) the ability to simulate large-scale transport patterns of radionuclides migrating in fracture networks from the repository to the biosphere. Two international collaboration activities have made great progress in addressing these challenges.

- Task G of the DECOVALEX-2023 initiative involved TM and HM modeling of single fracture mechanics exposed to complex stress states. Comparison of simulations conducted by national lab scientists with other international modeling teams showed that complex TM and HM experiments results could be well understood and reproduced numerically with sufficient accuracy representing main process characteristics. Micro-scale TM simulations of thermal shearing laboratory experiments identified the key properties impacting shearing behavior in flat and rough fracture surfaces. Modeling results of HM processes evaluated the effects of axisymmetric and triaxial loadings on the surface normal stress, surface displacement, and surface strain, and used these results to estimate hydraulic aperture and fracture permeability changes. The collaborative model comparison conducted in Task G will improve the reliability and predictability of models for fracture flow and transport in crystalline rock.
- Numerical modeling conducted under the umbrella of the SKB GWFTS Task Force focused on characterizing the impact of finite matrix block size on particle transport through fracture networks. It was shown that the travel time distributions through fracture networks with finite blocks are similar to those with infinite blocks when the fracture spacing is sufficiently large, matrix diffusion is relatively weak, or transport is considered at an early control plane distance. These results provide a first step toward developing a metric to assess when finite block size effects are expected to significantly influence transport, which could be critical for repository assessment.
- A new mesh generation methodology for 3D discrete fracture networks and the adjacent rock matrix (referred to as nMAPS) was developed, robustly tested, and integrated into LANL's powerful gridding toolkit. This new meshing capability will allow for better representation of geological features and repository structures to be included into GDSA PA simulations.

Progress Related to Coupled Processes in Salt (Section 6.6)

A broad portfolio of international collaboration has resulted in significant advances regarding understanding complex mechanical, hydrological, thermal, and chemical processes in salt.

- Collaborative research with German institutions included (1) assessing geotechnical barriers in salt in the collaborative project RANGERS, and (2) improving THM modeling for crushed salt (used as backfill for repository tunnels) in the joint KOMPASS and MEASURES projects.
  - The RANGERS Project completed a comprehensive compilation of existing knowledge and experience about geotechnical barriers in a salt repository. A key outcome of the work is a set of recommendations for designing and verifying geotechnical barriers based on the state of the art in science and technology.
  - The KOMPASS Project completed experimental investigations of microstructural effects on compaction methods and conducted a comparative THM model evaluation. Each modeling partner calibrated their model against laboratory tests performed on KOMPASS reference material, developed model improvements as necessary, and used the resulting calibrated model(s) to simulate the closure of a drift backfilled with crushed salt. Sandia began developing a new crushed salt constitutive model as part of the MEASURES proposal.
- International collaboration within the framework of Task E of the international DECOVALEX-2023 initiative allowed SFWST scientists to benefit from the engagement of international partners in the analysis and modeling of brine migration in heated salt. THM modeling conducted by the joint team of LBNL, SNL, and LANL researchers captured the main characteristics observed in the BATS heater experiment at WIPP, including modeling of the cooling-induced increase in brine inflow after heater turn-off and the evolution of damage in rock salt during heating and cooling. This work helped improve understanding of the complex processes expected to occur in the EDZ of a salt repository for disposal of heat-generating radioactive waste and supports building the long-term repository safety case for radioactive waste disposal in salt. Under leadership of SNL scientists, the collaborative salt modeling of recent BATS experiments continues in the current DECOVALEX-2027 phase.
- Under the umbrella of the NEA Salt Club, SFWST and international colleagues continued to develop a comprehensive FEPs database for salt host rock. They extended these efforts towards a generalized approach to scenario development for a high-level waste repository at a generic salt site.

Progress Related to the Hydromechanical Behavior of Faults and Fractures in Response to Repository-Induced Perturbation in Argillite Host Rock (Section 6.7)

Via field-based and simulation-based research, SFWST scientists made important advances in understanding whether and for how long faults and fractures in low-permeability host rock such as clay rock can be potential radionuclide migration pathways upon activation from repository-induced effects.

- SFWST scientists advanced the data and modeling analysis of the Mont Terri fault reactivation experiments to explore the ability of reactivated faults to self-seal over time. Integrating *in-situ* experiments and modeling revealed several key mechanisms contributing to the observed self-sealing phenomena following the activation of a shale fault. Time estimates for the return of a fault to its initial small transmissivity project a minimum of 50 years.
- Efficient ML approaches were developed for predicting fault reactivation processes, utilizing data from the 2020 fault reactivation conducted at Mont Terri. LBNL researchers tested a specific protocol for training the ML model, which ensures that the model can accurately represent the complex fault response both qualitatively and quantitatively during and after injection.

Progress Related to Characterization of Fractured Crystalline Rock (Section 6.8)

A key concern related to geologic disposal in fractured crystalline rock is the presence of potentially conductive fractures that could result in the transport of radionuclides. There is a need for improved hydrological, geomechanical, and geochemical techniques for the *in-situ* characterization of fractures including their hydromechanical properties and stress states.

- In cooperation with the COSC deep drilling project in Sweden, the deep borehole COSC-1 was used as a testbed for advanced site characterization of fractured crystalline rock. SFWST scientists developed and tested a new workflow using novel downhole probes to identify flowing fractures, evaluate their HM properties, and estimate the state of stress in the subsurface.
- Analysis of the COSC-1 data demonstrated that adding borehole displacement measurements to a standard hydraulic fracturing test allows for an accurate estimation of fracture HM properties (stiffness, hydraulic aperture), intact rock bulk and shear moduli, and local state of stress.
- To demonstrate that the SIMFIP deep borehole characterization workflow is mature, SFWST scientists recently deployed their method to characterize a crystalline host rock in the Bedretto URL (Switzerland), which provides straightforward access to a fault zone at a 1 km depth. Compared to the COSC-1 experiments in Sweden, the Bedretto tests highlighted that a fault zone may create significantly greater stress perturbations than single fractures. More experimental and interpretative work related to the Bedretto URL will be conducted in FY25.

Progress Related to Performance Assessment and Radionuclide Transport Modeling (Section 6.9)

Recognizing the importance of building confidence in the models, methods, and software used for PA of deep geologic repositories, SFWST researchers have increased their international collaboration in this area.

- In Task F of the DECOVALEX-2023 initiative, confidence in PA models and methods was enhanced by comparing PA modeling results from ten international disposal programs applied to the same reference cases, one involving a repository in a fractured crystalline host rock and another featuring a repository in a bedded salt formation. The comparison of PA approaches continues in the current DECOVALEX-2027 phase, with an enhanced focus on SA/UQ.
  - The crystalline reference case highlighted the importance of explicitly including drifts, buffer, and backfill in the simulations. For models with a comparable repository geometry and inventory evolution, the main source of model uncertainty was in the choices of how to represent the fracture network and simulate transport of two tracers. Overall, the modeling results showed considerable discrepancies and demonstrate the importance of examining multiple modeling approaches in PA.
  - Despite deploying different modeling strategies, all PA models for the salt reference case in Task F of DECOVALEX-2023 showed that the engineered barriers are effective for containing the radionuclides in the repository and that only a small amount of the disposed radionuclides will migrate beyond the repository seal over 100,000 years. All models also indicate that salt compaction and radionuclide diffusion are key physical processes in the simplified repository system.
- SFWST scientists play a key role in disseminating sorption data and acting as good data stewards by updating their improved database in a consistent format and assessing the quality of the newly assimilated data in an organized fashion. To this end, all data and workflows are open access and made available here: (https://seaborg.llnl.gov/resources/geochemical-databases-modeling-codes).

- Continued international collaboration of LLNL researchers within the NEA Thermochemical Database Project led to significant improvement in thermodynamic and thermochemical databases and models for radionuclide transport simulations. The goal is to produce interoperable open-source databases that harness modern data science workflows and algorithms.

Progress Related to Next Generation Workforce Development (Section 6.10)

Investing in the next generation of diverse, talented nuclear waste scientists and leaders is vital to fulfilling DOE NE's mission of developing solutions for the long-term geologic disposal of radioactive waste. In FY22, the SFWST program established a three-year Next Generation Workforce Development Pilot Program to attract, train, and advance a talented and diverse future workforce. LBNL and SNL started the program in FY22, and LANL was brought into the program in FY23. International collaboration is essential in this context. To help recruit and train a broad talent pool, the workforce development program has provided interesting learning/research challenges and attractive work-abroad opportunities in conjunction with SFWST's multiple international collaboration partners. While FY24 marks the final year of the three-year pilot, the program has been a great success and SFWST envisions continuation of the program into the foreseeable future.

- Stimulating Student Interest in Nuclear Waste Research: Between FY22 and FY24, the Next Generation Workforce Development Pilot Program has inspired many students via lab-university organized lectures and seminars to become interested in nuclear waste disposal science. In-person and hybrid lasses were held by national lab scientists at the University of New Mexico and the University of Puerto Rico ~ Mayaguez. A webinar series named "Next Generation Workforce Development for Spent Fuel and Waste Science and Technology" was co-organized by MIT, Texas A&M, SNL, and LBNL.
- Creating the Pipeline: Over the past three years, the summer internship program trained a large diverse student group of 29 interns at LBNL, SNL, and LANL. This clearly created a pipeline: Many of the summer interns returned to their hosting national lab (or other opportunities) after their initial summer program ended, either for another summer program or in some cases as year-round interns. At LBNL, three the summer interns were later hired as postdoctoral researchers.
- Advancing the Pipeline: LBNL and SNL each hired a dedicated "next generation" postdoc for a three-year research project with international collaboration, which allowed them to make remarkable research contributions. For example, LBNL's dedicated postdoc works on THM modeling for the international HotBENT Project and, to better connect her with the international community, participated in a 2023 summer training program at the Grimsel Test Site. SNL's dedicated postdoc works in GDSA Repository Safety Assessment (RSA), incorporating geology into UQ/SA.

SFWST scientists frequently present technical highlights from international collaboration activities at international conferences and symposia, to engage with the broader radioactive waste management and disposal sciences community, as well as with the other geoscience fields. They also play a leading role in organizing international conferences or conference sessions dedicated to geologic disposal research: For example, the First International DECOVALEX Coupled Processes Symposium, co-organized by SFWST researchers, was held in Brugg, Switzerland, in 2019 (http://decovalex-coupled-processes-symposium.org/), followed by the Second International DECOVALEX Coupled Processes Symposium held in Troyes, France, in 2023 (https://2023-decovalex-coupled-processes-symposium.lbl.gov/home). A session on international collaboration in disposal research was organized during the "International Conference on Coupled Processes in Fractured Geological Media – CouFRAC" (held in Berkeley, November 14-16, 2022) and focused on recent advances from the nuclear waste disposal field and many other applications; a session with a similar focus was recently held at the TOUGH Symposium 2023, also in Berkeley from September 18-20, 2023.

SFWST's international research activities are also a frequent topic at public meetings organized by the U.S. Nuclear Waste Technical Review Board (NWTRB). Most prominently, the April 2019 meeting in San Francisco was dedicated to "Recent Advances in Repository Science and Operations from International Underground Research Laboratory Collaborations". The workshop report developed by the NWTRB provides an excellent summary of international activities and the critical role of underground research laboratories (NWTRB, 2020). Other recent NTWRB public meetings with international activities in disposal research on the agenda are the December 2020 meeting with a focus on generic disposal research and development program and priorities; the November 2021 meeting with a focus on research and development activities related to the geologic disposal safety assessment framework; the September 2022 meeting with a focus on geologic disposal in clay-bearing host rocks and R&D on clay-based engineered barriers; and the May 2024 meeting with a focus on geologic disposal in crystalline rocks.

We note that the U.S. Nuclear Waste Technical Review Board (NWTRB) in FY21 released a report to the U.S. Congress and the Department of Energy entitled "Six Overarching Recommendations for How to Move the Nation's Nuclear Waste Management Program Forward" (NWTRB, 2021). One of the six recommendations is to continue and expand engagement with the international community, and to sustain active engagement in international programs given the tangible benefits derived from close involvement. The Board also recommended continuing and expand participation in collaborative international URL activities, which is a key goal of DOE's international collaboration activities in disposal research.

Going forward, international collaboration will continue to be an important cross-cutting campaign activity within the SFWST campaign, providing further opportunities for conducting *in-situ* experiments in underground research laboratories across a range of geologic systems. In FY20 and FY21, SFWST leadership discussed the 5-year direction of the campaign and developed a 5-year plan that serves as a strategic guide to the work within the disposal research R&D technical areas (i.e., the control accounts), focusing on the highest priority technical thrusts (Sassani et al., 2020; 2021; 2023). The plan defines a comprehensive list of near-term to mid-term goals for international collaboration as a central element of the campaign's disposal research (see summary in Section 5). There are ample opportunities to continue and even expand on the current portfolio of international research, several of which are mentioned in this report. The 5-year plan also discusses the importance of integrating international activities across all control accounts, including performance assessment modeling, where the joint modeling and comparative analysis of complex *in-situ* experiments can ultimately lead to better predictive models and thus directly contribute to the confidence building of PA predictions. As long-term topics, the plan identifies the potential value of international collaboration in (1) developing best practices and technologies for site selection and characterization and (2) utilizing international activities for the training/education of junior staff. The campaign has already acted on the latter item, as mentioned above, and seeks to pursue the former item in the next 3- to 5-years. International collaboration opportunities related to siting approaches and site characterization practices are identified throughout this report.

The 5-year plan in Sassani et al. (2020; 2021; 2023) furthermore calls for DOE to consider moving from a mostly participatory role in ongoing *in-situ* experiments conducted by other nations to a more active role in conducting its experimental program in international URLs. The advantage of active planning is that the experimental focus and design can be better tailored to the campaign's needs. Some collaborative initiatives like the Mont Terri Project provide their partner organizations with the opportunity to conduct their experimental work and invite other partners to join. This option would allow the U.S. disposal program to lead targeted *in-situ* field activities in representative host rocks, even though there are currently no operating underground research laboratories in clay or crystalline host rock environments in the U.S.

While there are no immediate plans for DOE to conduct its experiments in international URLs, SFWST's disposal program has already started taking a much more active approach in shaping the future R&D portfolio of the international initiatives it has joined as a partner. For example, with Jens Birkholzer of LBNL as Chair of the international DECOVALEX Project, SFWST scientists have been instrumental in the definition and selection of tasks for the current DECOVALEX-2023 initiative, and are now leading two of the seven modeling tasks, one focusing on the BATS heater test at WIPP, and one comparing different performance assessment approaches. In addition, DOE has co-developed with international partners the planning and design of the HotBENT Project, the full-scale high-temperature heater experiment at the Grimsel Test Site that entered its operational phase after several years of planning and construction. SFWST scientists also play a more active and leading role in the SKB EBS Task Force. By establishing a Center for International Collaboration in Disposal Research, SFWST currently considers elevating international collaboration in disposal research to a new level of emphasis and recognition.

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