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# DECOVALEX-2023: An International Collaboration for Advancing the Understanding and Modeling of Coupled Thermo-Hydro-Mechanical-Chemical (THMC) Processes in Geological Systems

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## Abstract

The DECOVALEX initiative is an international research collaboration ([www.decovalex.org](http://www.decovalex.org)), initiated in 1992, for advancing the understanding and modeling of coupled thermo-hydro-mechanical-chemical (THMC) processes in geological systems. DECOVALEX stands for “DEvelopment of COupled Models and VALidation against EXperiments”. The creation of this international initiative was motivated by the recognition that prediction of these coupled effects is an essential part of the performance and safety assessment of geologic disposal systems for radioactive waste and spent nuclear fuel. DECOVALEX emphasizes joint analysis and comparative modeling of the complex perturbations and coupled processes in geologic repositories and how these impact long-term performance predictions. The most recent phase of the DECOVALEX Project, here referred to as DECOVALEX-2023, started in early 2020 and ended in late 2023. More than fifty research teams associated with 17 international DECOVALEX partner organizations participated in the comparative evaluation of eight modeling tasks covering a wide range of spatial and temporal scales, geological formations, and coupled processes. This Virtual Special Issue on DECOVALEX-2023 provides an in-depth overview of these collaborative research efforts and how these have advanced the state-of-the-art of understanding and modeling coupled THMC processes. While primarily focused on radioactive waste, much of the work included here has wider application to many geoenvironmental topics.

## 1. Introduction

An important part of the safety assessment of disposal systems for radioactive waste and spent nuclear fuel in deep geological formations is to evaluate the impact of the coupled effects of mechanical deformation, fluid and gas flow through the repository, and thermal loading from the decaying waste. It has long been recognized that safety assessments for geologic radioactive waste disposal sites need to cognizant of such coupled processes, and hence there was a need to rigorously enhance the theoretical background and to develop models capable of simulating coupled thermo-hydro-mechanical (THM) processes<sup>1</sup>. More recently, chemical processes have also been added to enable the study of fully coupled THMC processes in geosystems.

The term "coupled processes" implies that each process potentially affects and is affected by the initiation and progress of all other processes<sup>2</sup>. Thus, the response of a rock mass to radioactive waste storage cannot be predicted with confidence by considering each process individually or in direct succession. In the field of rock mechanics and rock engineering, many studies have been made on two-way couplings TM and HM, but for predicting the repository performance, it is essential to study and be able to predict processes with THM

coupling, and even full THMC coupling<sup>3</sup>. Such coupling remains a major challenge to the science and engineering community, in part because relevant effects need to be better understood and described with constitutive relations, but also since the processes have widely different characteristic temporal and spatial scales. Coupled processes of course are not only relevant to geologic disposal of radioactive waste<sup>4</sup> but also play a critical role in a range of other sub-surface engineering activities<sup>5</sup>, such as carbon dioxide sequestration, enhanced geothermal systems, energy storage, as well as unconventional oil and gas production through hydraulic stimulation.

In 1992, recognizing the need to address the modeling challenges related to coupled THM and (in later stages) THMC processes, DECOVALEX was initiated as an international cooperative project of radioactive waste management organizations, regulatory agencies, research institutions and academia involved in various national programs, providing a wide range of perspectives and solutions to these complex problems. Analysis and comparative modeling of state-of-the-art field and laboratory experiments has been at the core of the collaborative work, with an increasing focus on characterizing uncertainty and blind prediction of experimental results and translating the predictions of complex coupled processes into long-term safety assessments.

DECOVALEX has been operating in four-year phases, each phase featuring a number (typically three to seven) of modeling tasks. Seven phases were successfully concluded between 1992 and 2019, results of which have been summarized in overview publications<sup>1,6-10</sup> and 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, Vol. 42(5-6) in 2005, and a Virtual Special Issue in 2021), 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), and in a 2018 Topical Collection “DECOVALEX-2015” in the Journal of Environmental Earth Sciences.

The 8<sup>th</sup> phase of the DECOVALEX project, here referred to as DECOVALEX-2023, comprised of more than 50 modeling teams associated with 17 international partner organizations, which participated in the comparative evaluation of eight complex modeling tasks (i.e., Tasks A through F1 and F2). Together, these tasks address a wide range of relevant issues related to engineered and natural system behavior in a variety of potential host rocks, including clay rocks, crystalline rocks, and bedded salts. The 44 publications in this Virtual Special Issue provide an in-depth overview of the collaborative research efforts conducted in each task and how these have advanced the state-of-the-art of understanding and modeling coupled THMC processes. Below, we briefly introduce each task and provide references to respective publications. One of the most important characteristics of DECOVALEX is the emphasis on a cooperative research environment and the desire to gain insight by comparative analysis of multiple alternative approaches. This characteristic is reflected by jointly authored synthesis papers for each task. These provide an overview of the modeling approaches pursued by individual research teams and discuss which concepts and models have been particularly suited for a given coupled problem. The 10 synthesis papers are supplemented by 33 detailed publications describing the research methods and findings of individual teams participating in the eight tasks. While not explicitly conducted within DECOVALEX-2023, this Virtual Special Issue comprises one additional paper<sup>11</sup> from a previous DECOVALEX phase, which explores the impact of a thermal gradient and coupled THM processes on solute migration in clay rock, using data from a laboratory diffusion experiment and an ongoing *in situ* experiment on solute transport under a thermal gradient at the Tournemire underground research laboratory (URL) in Southern France. This work has sufficient overlap with the other DECOVALEX efforts and was judged appropriate to include in the special issue.

## 2. DECOVALEX-2023 Tasks

The seven DECOVALEX-2023 tasks can be grouped into three general themes:

- Basic Understanding of Safety-Relevant Coupled Processes (Tasks A, B, E, and G)
- Full-Scale Demonstration Experiments of Disposal Systems (Tasks C and D)
- Safety Assessment Models and Methods (Tasks F1 and F2)

The tasks under each theme are briefly introduced below.

### 2.1 Basic Understanding of Safety-Relevant Coupled Processes

#### Task A: HGFract - Heat and Gas Fracturing in Clays

The overall objective of Task A was to improve the ability of models to predict the processes and mechanisms of fracture initiation and growth in clay host rock due to a strong increase of heat or gas overpressure. Such thermal or fluid pressure perturbations can be expected in a radioactive waste repository, caused by respectively the emplacement of heat-emanating waste and the gas production due to the corrosion of metals, including steel canisters and other metallic components, and the microbial degradation of organic waste. Based on heat and gas fracturing *in situ* experiments conducted at the Bure URL in France, HGFract enhanced the understanding of fundamental fracturing processes and improved capabilities for numerical modeling of these processes. Several tests had been designed and conducted at Bure to reach the rupture of claystone under either a rapid heat load or substantial gas pressure increase. The task was divided into two 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, and (3) application at the repository scale.

For heat-driven fracturing, the modeling steps started with simulating laboratory triaxial extension tests, which featured a fast-heating phase and an automatic confining control under constant vertical total stress. 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 1). Accordingly, the six participating research teams first simulated the laboratory thermal extension tests conducted on Callovo-Oxfordian claystone (COx) samples, and 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 mechanical approaches, including continuum and discrete methods, to model these two tests: thermo-poro-elasticity, elasto-plasticity, phase field methods, and weak planes modeled as Mohr-Coulomb joints, both explicitly and implicitly. Failure criteria for their respective THM models were defined through the laboratory tests. 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 the general thermal-hydro-mechanical evolution of the system. Teams initially overestimated pore pressure in the heated zone but were able to address this issue by considering an explicit excavation-induced fracture network around the heater boreholes (Figure 2). Thermal fracture initiation in the COx was well represented by the models in terms of time of occurrence and location, based on respective stress analyses, whereas attempts to reproduce fracture aperture or fracture propagation were less accurate and will require more work in the future. A summary of the collaborative research work conducted in this thermal fracturing task is given in the synthesis paper by Plúa et al.<sup>12</sup>, complemented by additional publications from individual research groups simulating the laboratory extension tests and the CRQ field experiment<sup>13,14,15</sup>. Other researchers<sup>16,17</sup> expanded the thermal fracturing predictions to evaluate failure potential at the repository scale.

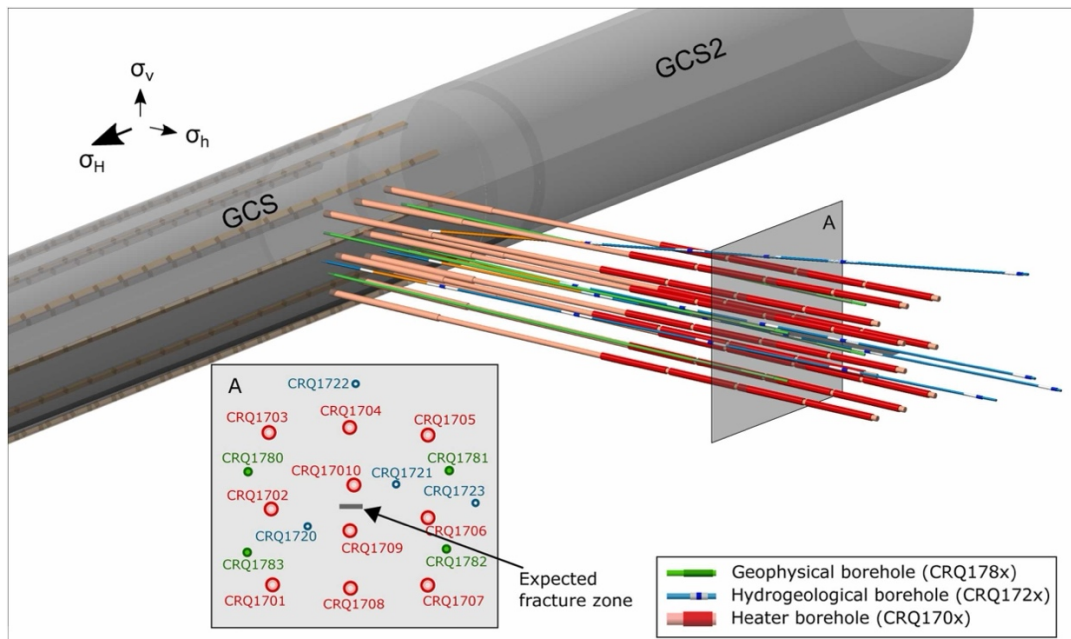


Figure 1. Layout of the CRQ thermal fracturing field experiment in the Bure URL in France and cross-section at the mid-plane of the heaters (i.e., 15 m from the GCS drift wall)<sup>12</sup>

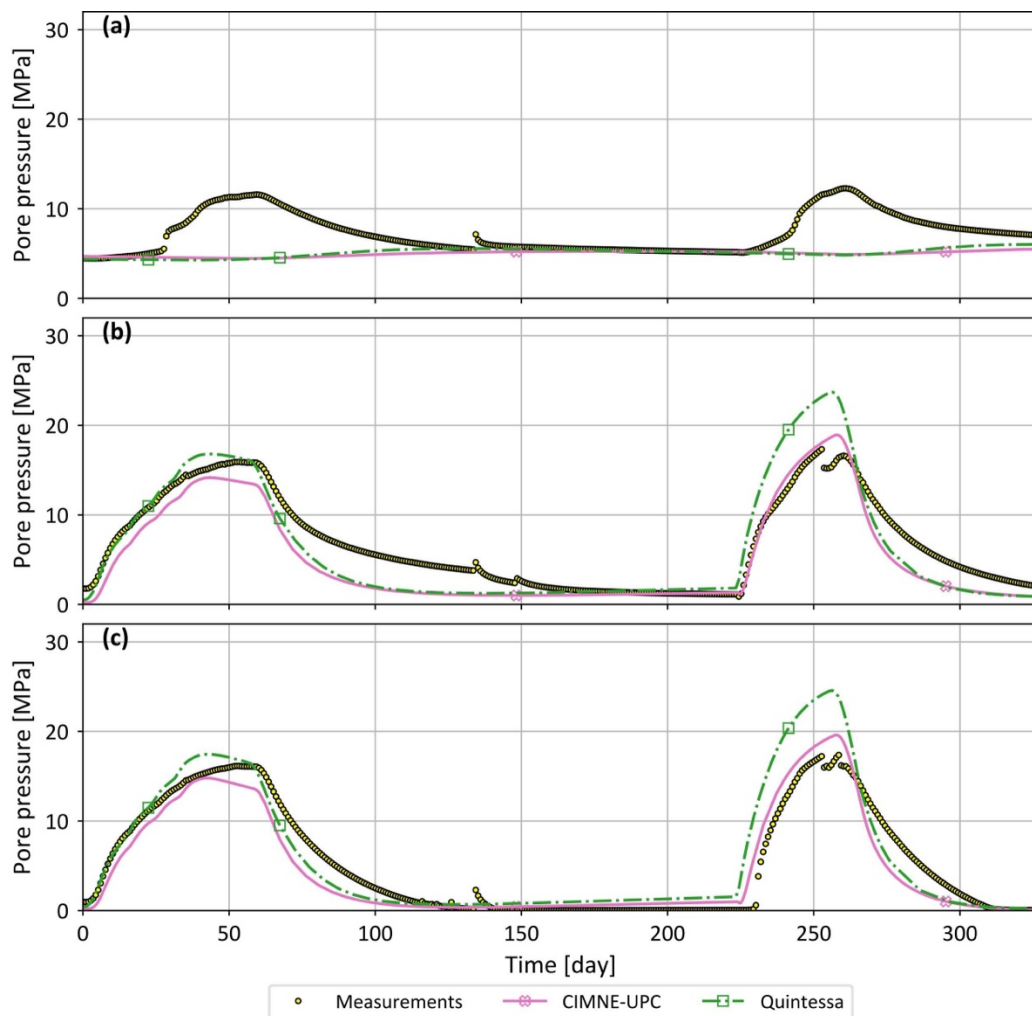


Figure 2. Comparison of numerical results obtained with an explicit excavation-induced fracture network around the heater boreholes and pore pressure measurements: (a) CRQ1720\_01, (b) CRQ1720\_02, and (c) CRQ1720\_03, from<sup>12</sup>

The task on gas-pressure-driven fracturing focused on a series of *in situ* gas injection experiments (PGZ) performed at the Bure URL (Figure 3). These tests used a multi-packer system installed in two small diameter boreholes drilled in the clay host rock, one parallel and one perpendicular to the principal stress direction. Gas injection into the packed-off interval consisted of several phases, the first of which aimed to generate a fracture, while subsequent phases aimed to reopen the fracture and identify the fracture closure pressure. Three research teams participated using three distinct numerical approaches: a viscoplastic model with Mohr-Coulomb failure and softening, a hydromechanical damage model based on the phase-field method, and a model combining a failure index with dilatancy-dependent permeability. 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. First, the research teams investigated the impact of gas migration and fluid pressurization within the COx claystone and the fracturing threshold pressure through a series of benchmark exercises of increasing complexity (Figure 4). Then the research teams used their models to reproduce two gas injections conducted in the PGZ field test. Overall, the numerical simulations yielded acceptable results and provided insights into the hydromechanical response of the Bure 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 reproducing the *in-situ* tests. The multiple approaches adopted in this task showed promising results as they could explain the observed fracture development under certain conditions. A summary of the collaborative research work conducted in this gas fracturing task is given in the synthesis paper by Plúa et al.<sup>18</sup>. Additional papers provide results from individual modeling groups on the benchmark tests<sup>19, 20, 21</sup> and the PGZ field experiment<sup>22</sup>.

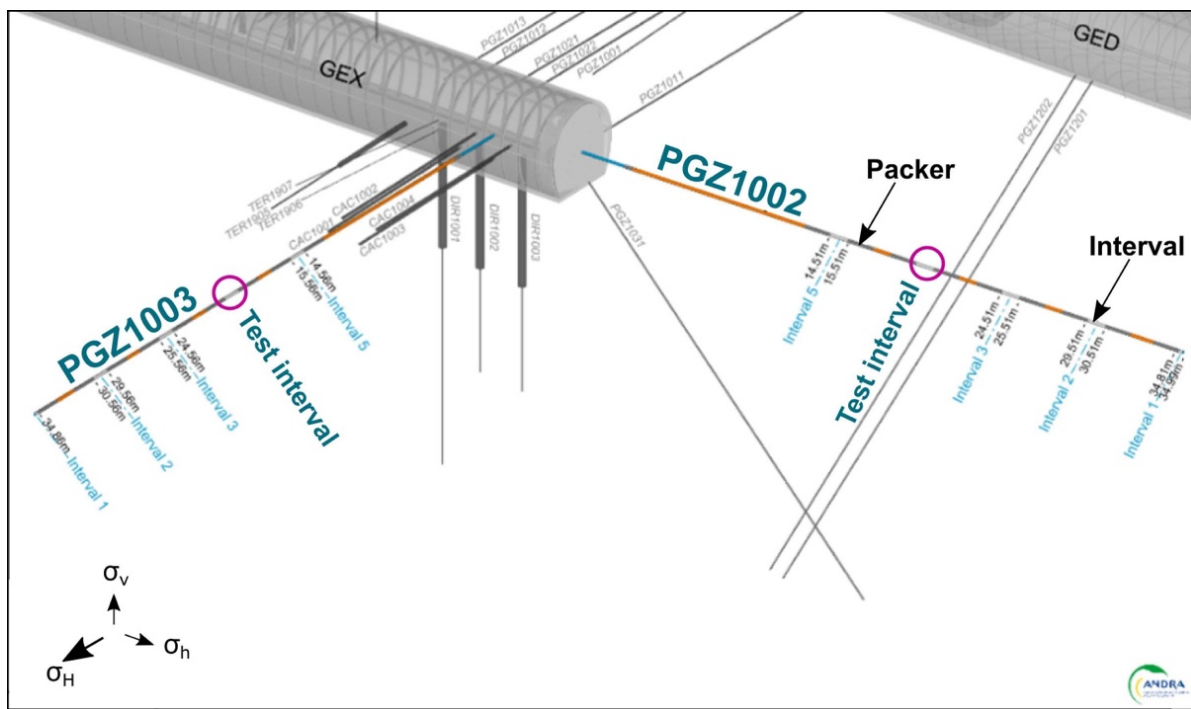


Figure 3. Layout of the PGZ gas injection field experiment in the Bure URL in France<sup>18</sup>

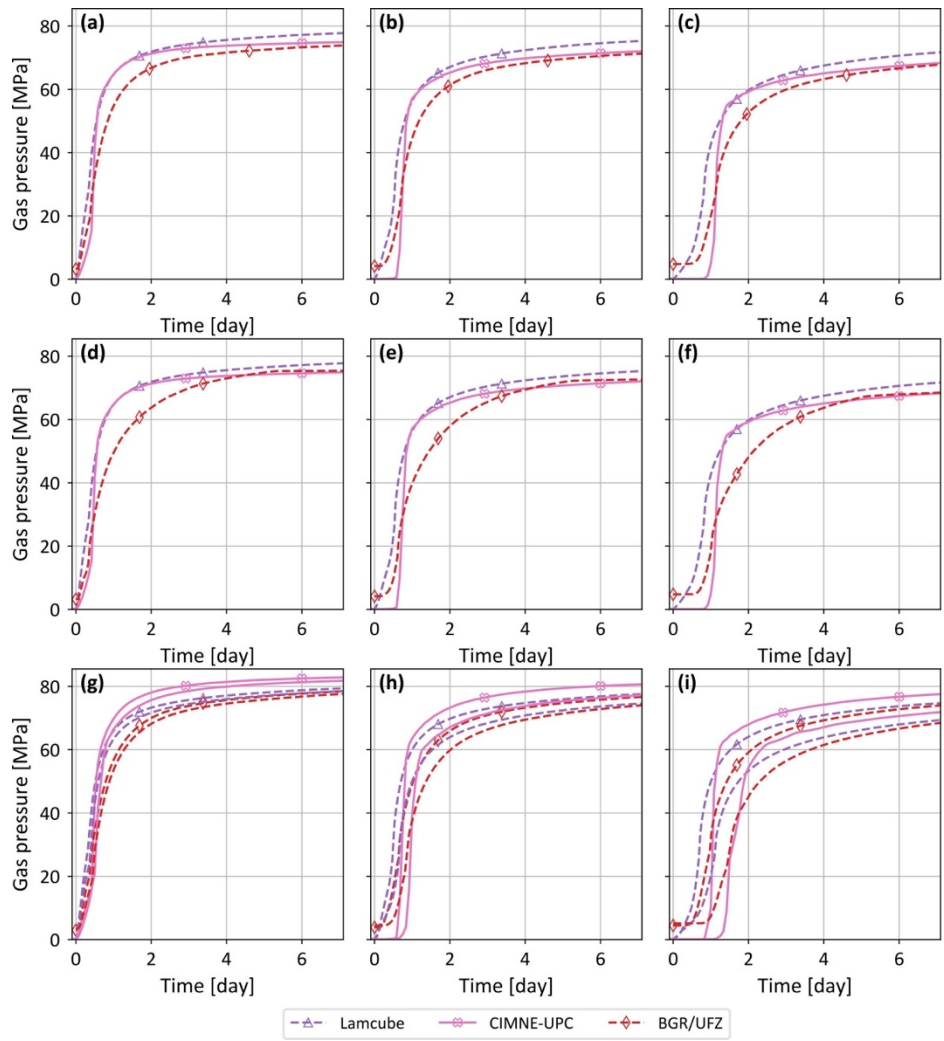


Figure 4. Evolution of gas pressure for Benchmarks B1, B3, and B5. These benchmarks were designed to capture processes related to gas diffusion under the framework of poroelasticity. Points in the horizontal direction with markers and points in the vertical direction without markers.<sup>18</sup>

#### Task B: MAGIC - Modeling Advection of Gas in Clays

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 ultimately support the development of performance and safety assessment models. As an extension of a related modeling challenge from a prior DECOVALEX phase which was based on data from well-instrumented laboratory tests, MAGIC centered on the Large-Scale Gas Injection Test (LASGIT), a field experiment conducted at the Äspö Hard Rock Laboratory in Sweden. LASGIT comprised a mock waste canister encapsulated in bentonite placed within a vertical deposition hole in a granitic host rock (Figure 5). The bentonite was allowed to hydrate since 2005 after a 2-year construction phase ended with the closure of the deposition hole. Subsequently, gas injection tests have been conducted occasionally from several filters embedded along the surface of the canister. The test was highly instrumented: Sensors continually monitored 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.

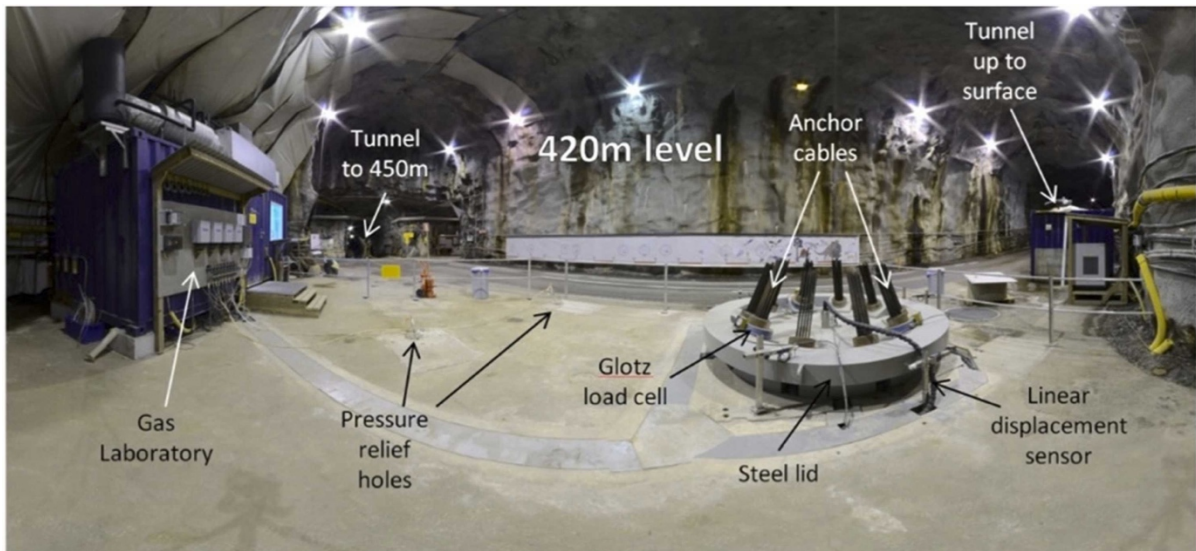


Figure 5. A panoramic view of the Large-scale gas injection test (Lasgit) 420 m below ground at the Äspö Hard Rock Laboratory in Sweden, from<sup>28</sup>. The blue container on the left housed the artificial hydration and gas injection systems which were connected into the borehole along channels cut into the gallery floor. The lid and rock anchors of the deposition hole can be seen in the center right.

Task B modeling activities were conducted in two subsequent steps. The first step, summarized in the synthesis paper by Tamayo-Mas et al.<sup>23</sup>, involved the development of enhanced numerical representations of key processes for gas migration and compared the performance of each against high-quality laboratory test data. The experimental data revealed that gas percolation in water-saturated compacted bentonite is characterized by four key features: (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. Most of the research teams participating in Task B applied hydromechanical models based on the multiphase flow theory, which provided good initial values and reasonable responses for gas breakthrough and peak gas pressure values<sup>24,25,26</sup>. To further understand gas flow localization, a new conceptual model was developed by one of the teams, which shows that discrete channels 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<sup>27</sup>.

In the second step, modeling teams deployed the most successful modeling approaches from laboratory-scale modeling to the LASGIT field experiment (Figure 6). As discussed in a second synthesis paper<sup>28</sup>, 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 minor adjustment of some parameters, the upscaled and partially updated models were able to represent most of the key features observed in the experimental data, even at a large scale. Detailed results from individual modeling groups simulating the LASGIT field experiment can be found in<sup>25,29,26</sup>.

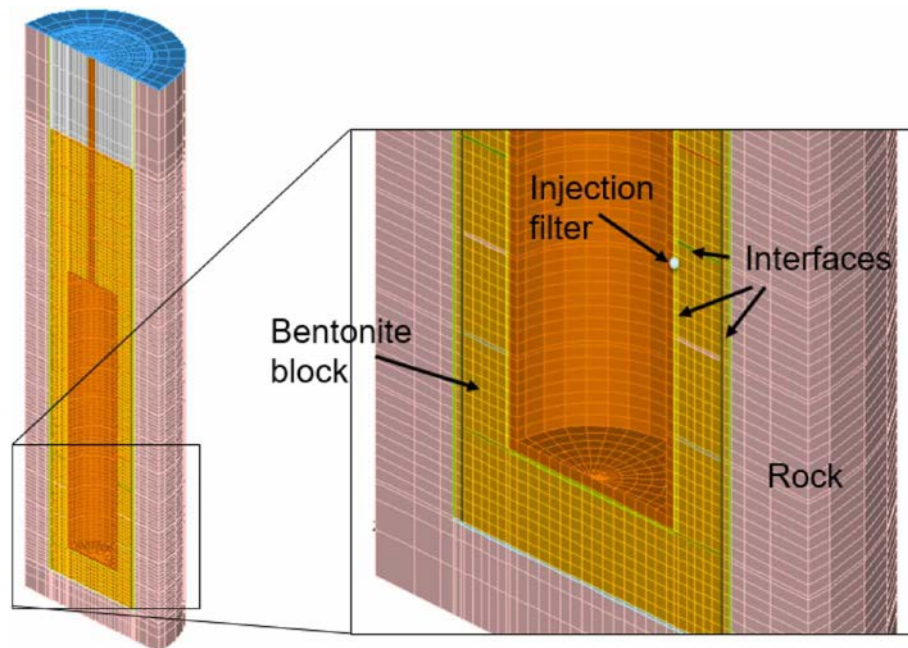


Figure 6. Example of a half-symmetric 3D model used to describe the Lasgit experiment, from<sup>28</sup>. To represent the potential for flow along engineered barrier and host rock interfaces, this model had designated interface elements between (1) bentonite blocks, (2) the canister and the bentonite, and (3) the crystalline host rock and the bentonite.

#### Task E: BATS – Brine Availability in Salt Experiment

The objective of this task was to jointly predict the coupled processes governing water movement in response to a strong heat source emplaced in a bedded salt formation. Brine availability has the potential to strongly impact the long-term performance of salt repositories for heat-generating radioactive waste. Brine can lead to the corrosion of waste forms and packages, generation of gas, and the possible dissolution of radionuclides, with brine and gas transport being a potential transport vector to the accessible environment. The task utilized data from the BATS experiments 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) in New Mexico, USA<sup>30</sup>. The boreholes were arranged in two separate adjacent arrays of 13 parallel monitoring boreholes each, drilled horizontally into the tunnel wall. One array includes a central heated borehole (Figure 7) while the unheated array serves as an unheated control. The experimental observations allowed the types and strengths of coupled THMC process interaction to be characterized and hence gave insight into potential brine flow paths and canister corrosion. The data from BATS therefore provided a unique opportunity to validate numerical and constitutive models for coupled processes and salt migration in bedded salt.

As summarized in the synthesis paper by Kuhlman et al.<sup>30</sup>, Task E was structured into several steps that increased in complexity and realism, beginning with historical single-phase unheated brine inflow ( $H^1$ ) and heat conduction (T), followed by simplified benchmarking of coupled thermal, mechanical and multi-phase flow processes (TH<sup>2</sup>M) in salt, and ending with interpretative modeling of brine migration from the BATS experiment and comparison against the observed brine inflow behavior. The eight modeling teams participating in Task E came to the problem with a range of modeling tools and conceptual approaches. Given the complexity of the problem, some teams used one- or two-dimensional models of the thermo-mechanical and brine migration processes, while others included more geometrical fidelity in three-dimensional models (Figure 8). The collective modeling of brine inflow conducted by teams from the USA, UK, and Germany led to an increased understanding of the complex behavior expected to occur in the EDZ of a salt repository for the disposal of heat-generating radioactive waste. Most models were able to tease out the following characteristics of the BATS experiment, namely that (1) permeability is higher near the borehole/excavation, caused by the effects of excavation damage, (2) fluid pressure is highest at the end of heating, due to thermal pressurization, and (3) permeability increases at the end of heating due to thermal contraction and tensile stresses developing near

the borehole, which allows the elevated fluid pressures to quickly dissipate. Construction of fully coupled models accounting for all the process couplings in a single model, while was extremely complex, was attempted with some success by a sub-set of teams. Detailed results from individual modeling groups simulating the BATS experiment can be found in<sup>31,32,33</sup>. Complementing these field-scale models, Wang et al.<sup>34</sup> presented a new theoretical framework for modeling fluid flows in deformable low-permeability media like salt.

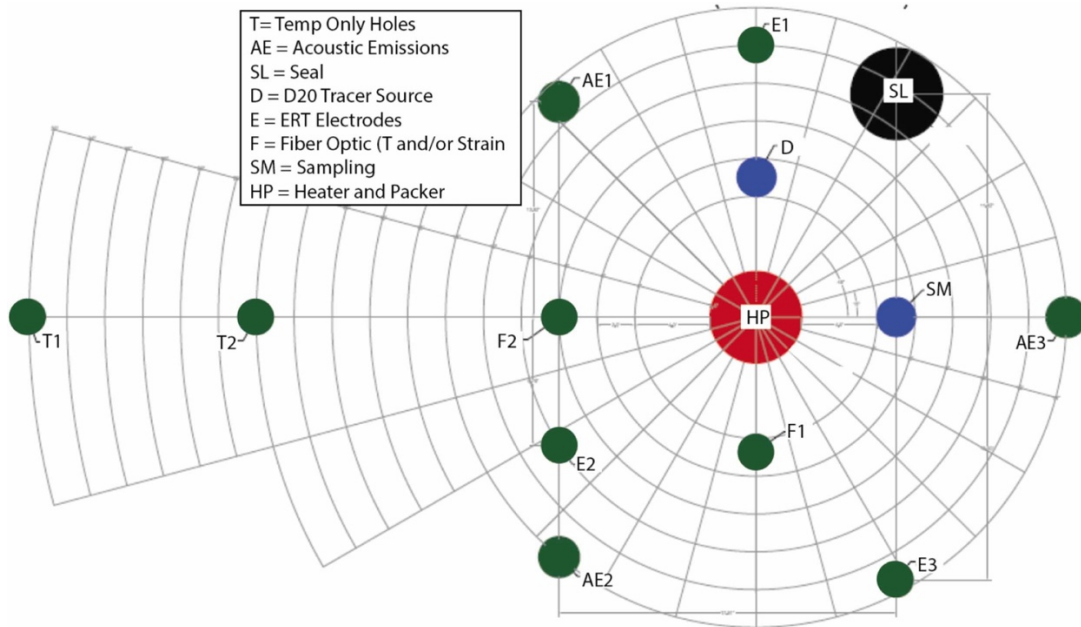


Figure 7. Borehole layout for BATS experiment showing the array of boreholes on the wall of the experimental drift in the WIPP facility in the US, from<sup>30</sup>.

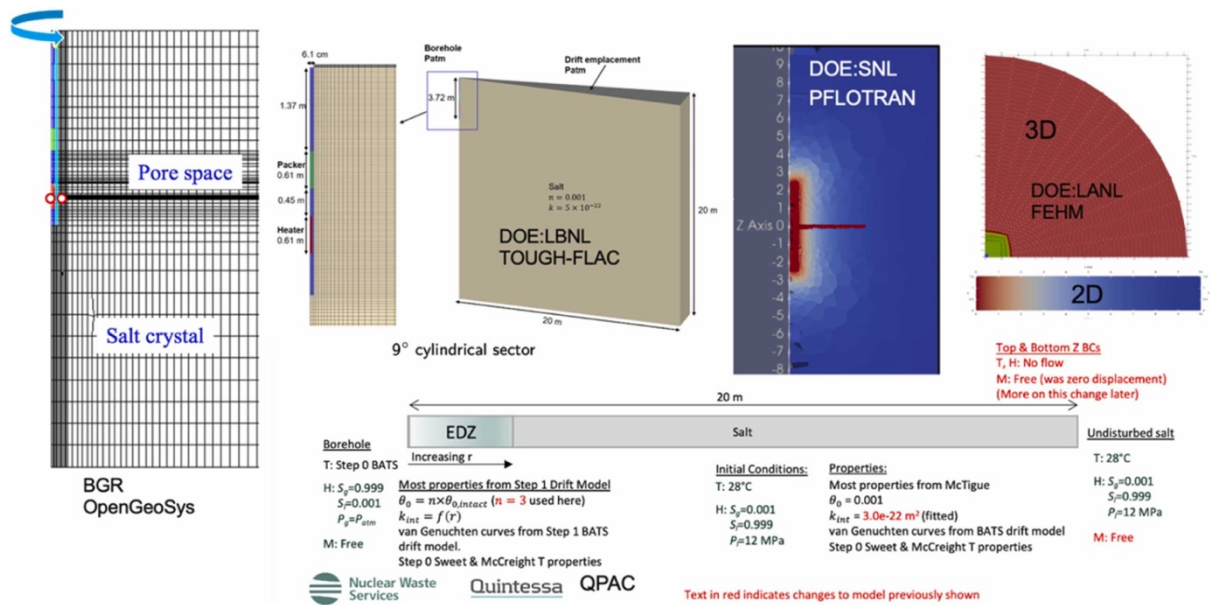


Figure 8. Conceptual models used by the participating teams to simulate the BATS heated brine flow, from<sup>30</sup>. One team used a one-dimensional conceptualization, three teams used two-dimensional conceptualization, and two teams used 3D conceptualizations.

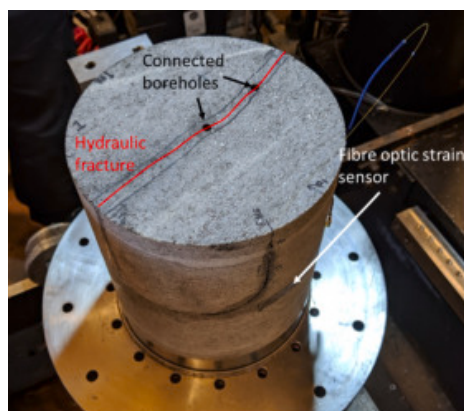
A significant amount of learning occurred both within and between teams, as different modeling approaches were attempted, modified, and sometimes dropped<sup>27</sup>. The primary lessons learned were the important effect of hydrologic initialization methods to describe the initial conditions, the difference between confined and unconfined thermal expansion, and the significant changes in permeability associated with heating and cooling.

Feedback and lessons learned during the modeling of BATS in DECOVALEX-2023 have also led to changes in the design and execution of follow-on BATS experiments.

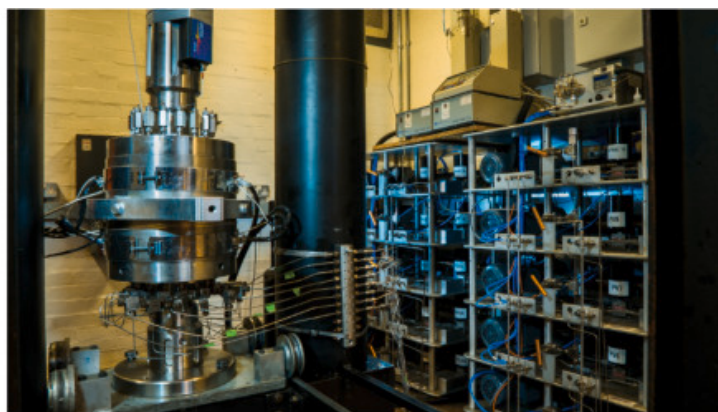
#### Task G: SAFENET - Micro-Scale THMC Lab Experiments with Focus on Shear

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 modeling challenges related to core-scale laboratory experiments<sup>35</sup>, as follows:

- Step 1: 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. This step elucidated the mechanics of rough fractures and how they were affected by shear and normal displacement.
- Step 2: Investigation of hydromechanical (HM) laboratory test results obtained with a unique triaxial test cell that creates a truly polyaxial rotatable stress field in large core samples (GREAT cell – Figure 9). Building on Step 1 and using the same rock samples, this step focuses on fundamental shear processes under complex 3D stress states, elucidating HM controls on fracture fluid flow under repository *in-situ* conditions, based on measurements of deformation, fracture normal stress, shear stress, and fluid pressure.
- Step 3: Investigation of thermo-mechanical (TM) laboratory test results obtained from triaxial testing of shear processes in fractured samples exposed to thermal stresses. Building on Step 1 and run in parallel with Step 2, this step investigated whether long-term heating effects can induce the shear slip of a stressed fracture, and, if so, what factors control the shear slip process.
- Step 4: Creative thinking by the teams on combining the developed approaches and upscaling to address larger scale applications.



(a) Sample preparation



(b) Experimental facility

Figure 9. The GREAT cell is a flexible-medium true-triaxial deformation rig for THMC investigation on large laboratory-scale sample, from<sup>35</sup>.

Eight international modeling teams collaborated to simulate and predict the M, HM, and TM response of fractured rock exposed to repository-induced perturbations<sup>35</sup>. The teams used a variety of different numerical methods comprising continuum, discontinuum, and hybrid approaches. 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 the 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 M, HM and TM experiments results could be better understood and reproduced numerically with sufficient accuracy representing the primary process characteristics.

Most modeling teams started with benchmark simulations to set the stage for more complex predictive and interpretative modeling of the laboratory experiments. Hu et al.<sup>36</sup> compared modeling results for three different fracture benchmarks that involved different levels of complexity of intersecting fracture. The overall agreement between different codes and software demonstrated that, for these benchmarks, shearing processes in discrete fracture networks could be adequately represented by continuum, discontinuum as well as hybrid methods. Modeling analysis of the laboratory experiments demonstrated that, based on the developed methodology and cross-comparison of simulation results between multiple teams, the experimental results could also be reproduced with reasonable accuracy, representing the primary process characteristics and elucidating M, HM and TM controls on shearing. By systematically investigating first the mechanical and then the hydro- and thermo-mechanical processes, the influence of individual coupled processes could be precisely quantified. Here are some major findings from the SAFENET task as summarized in<sup>35</sup> and further detailed in individual modeling team papers<sup>37,38,39</sup>.

- The Step 1 mechanical 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 and interpretative modeling, 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 hydro-mechanical experiments collected high-resolution strain data in variable polyaxial stress fields and determined the stress-dependent fracture permeabilities. The joint modeling analysis in this task improved the understanding of permeability changes during stress redistributions, e.g., when excavating cavities in crystalline hot rock (Figure 10).
- The Step 3 thermo-mechanical experiments and their TM modeling interpretation evaluated under which conditions thermal shearing can occur and what the controlling factors are. Thermal shearing may play an important role for repository safety because strong temperature increases can be expected due to the storage of heat-generating waste.

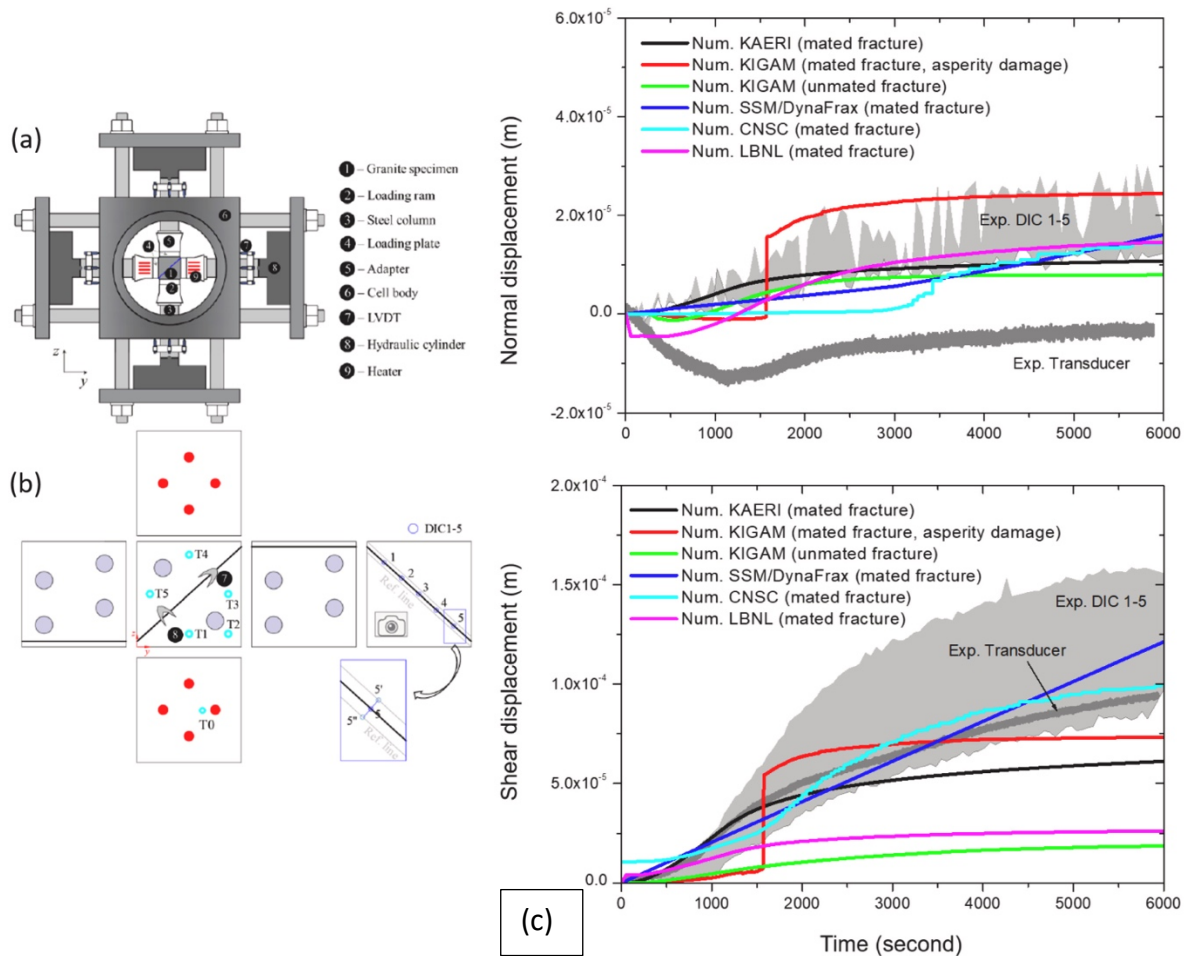


Figure 10. Shear slip experimental setup and results from KICT, from<sup>35</sup>. The schematic diagrams on the left show the locations of heaters, clip-on gages, thermocouples, and AE sensors (a) from the full front view and (b) on the six square faces of a cube. On the back side of the specimen, a camera was used to take photos of the back side for DIC analysis, and the fracture slip and shear dilation at the five locations (labeled 1–5) were indirectly measured. Simulation results for the tensile-split rough fracture test and comparison with the experimental data are shown in (c) on the right. The DIC data range is plotted as gray zone and the transducer measurement is plotted as a dark curve.

## 2.2 Full-Scale Demonstration Experiments of Disposal Systems

### Task C: THM Modeling of the FE Experiment at the Mont Terri URL

This task aimed to model THM processes in the Opalinus Clay host rock using measurements from the Full-Scale Emplacement (FE) Experiment at the Mont Terri URL in Switzerland, a mock-up of the Swiss disposal concept (Figure 11). One of the motivations for this experiment was to provide data for validation of existing THM models, at the full scale for geological disposal. The heating phase of the experiment started in 2015 after a few years of tunnel construction and three years of ventilation. Data provided to the participating modeling teams included pore pressure, temperature, relative humidity, displacement and inclination measurements, obtained at high spatial and temporal resolution during the construction, ventilation and ongoing heating phases. The specific focus of Task C was to understand the pore pressure evolution in the host rock in response to the strong thermal perturbation and how this response is affected by engineering factors (e.g., shotcrete for tunnel support, tunnel shape) and damage due to tunnel construction. Task C was structured into several steps, starting with a preparation and benchmarking phase, followed by modeling of the FE heating phase, and finally, modeling of the FE ventilation phase.

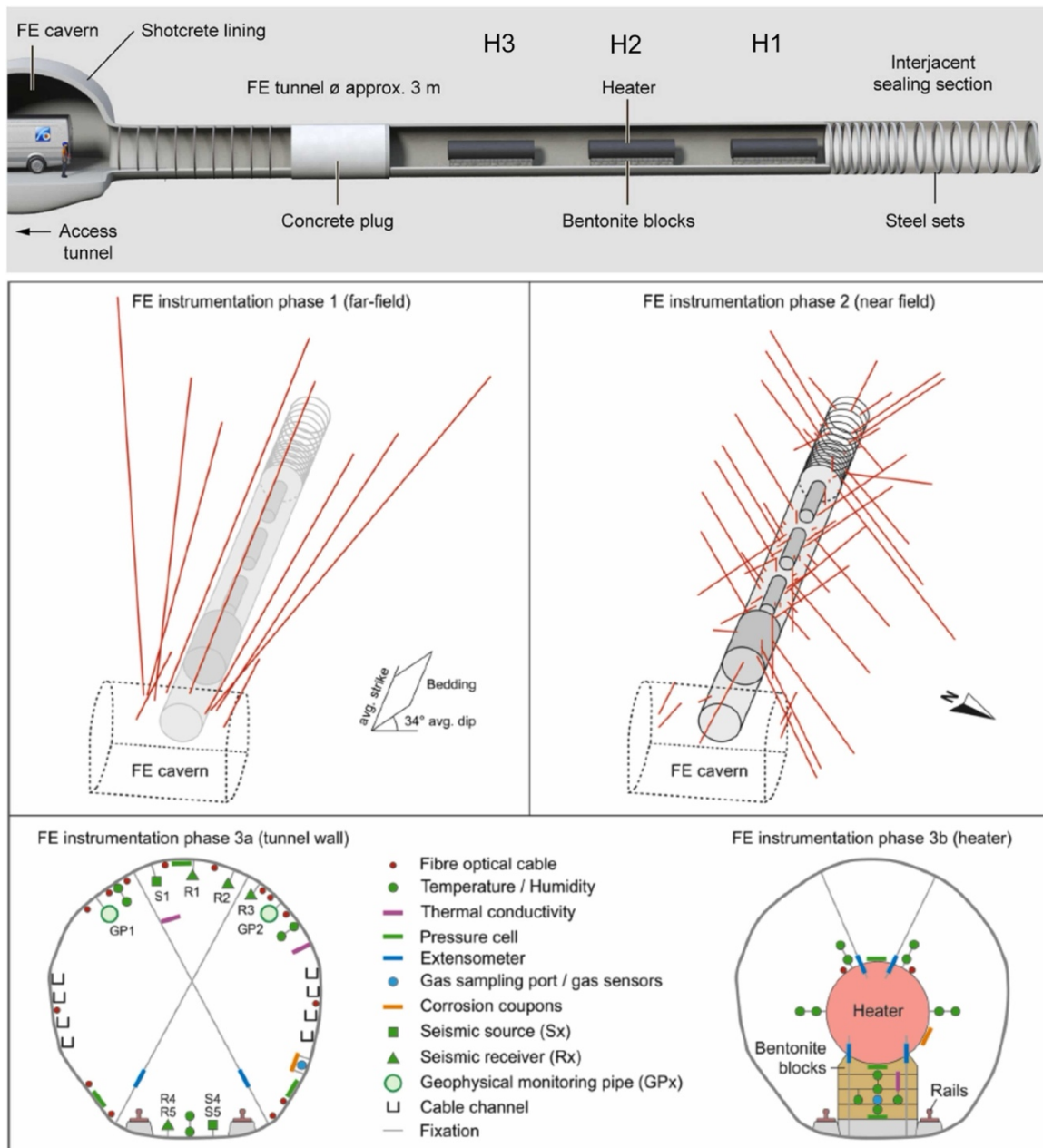


Figure 11. Experimental layout (top) and measurements (bottom) from the FE Experiment in the Mont Terri URL in Switzerland, from<sup>40</sup>.

As summarized in the synthesis paper by Graupner et al.<sup>40</sup>, nine modeling 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. The rather extensive benchmark studies conducted beforehand provided an important test before undertaking the full complexity of the *in situ* experiment. 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<sup>40</sup>. 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 drying-out effect. Modeling the pore pressure evolution was more complex because it

comprises the entire interaction of the coupled THM processes. The spread between the pore pressure modeled by the teams was larger, 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 as distance increased away from the heater (Figure 12). It was concluded that the excavation damage zone and the shotcrete could influence the behavior of the rock near the tunnel, causing larger differences closer to the heater. Further research will be needed to implement those influences into the models better. Kaiser et al.<sup>41</sup> conducted a systematic evaluation of several modeling choices and their impact on modeling results (among them geometrical aspects as aspects of model complexity such as inclusion of engineering features or coupled processes), providing a valuable basis for model improvement. Kim et al.<sup>42</sup> investigated capillary effects in the bentonite on the disposal system. Their analysis revealed that strong capillary suction significantly influenced the pore pressure change in the host rock near the tunnel, while thermal pressurization became dominant with increasing distance.

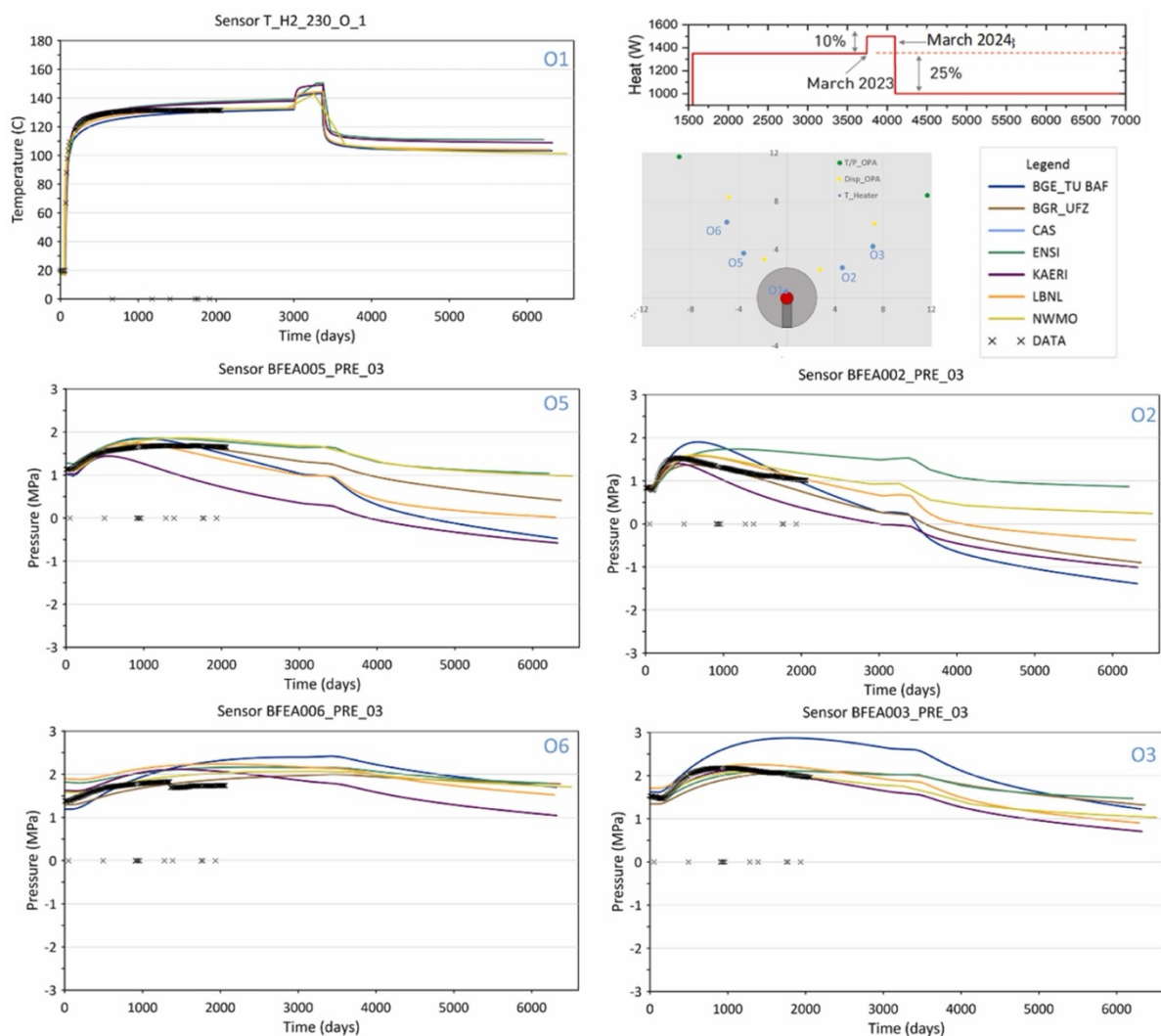


Figure 12. Comparison of pore pressure modelling results versus the experimental data from the FEEperiment, from<sup>40</sup>.

#### Task D: Full-scale Engineered Barrier System Experiment at the Horonobe URL

The objective of this task was to better understand, simulate and interpret the coupled THM processes occurring in and around an engineered barrier system (EGS) as designed in the Japanese disposal concept<sup>43</sup>. The EBS Experiment at the Horonobe URL in Japan 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 (Figure 13). 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 to monitor the coupled THM processes, including temperature, total pressure and pore pressure, water content, resistivity, displacement, and strain. After some initial benchmarking, the task comprised two main modeling steps for: The first step involved modeling several laboratory tests using buffer and backfill materials (swelling tests, hydraulic tests, moisture diffusion tests under thermal gradient), followed in the second step by simulating the full-scale EBS Experiment.

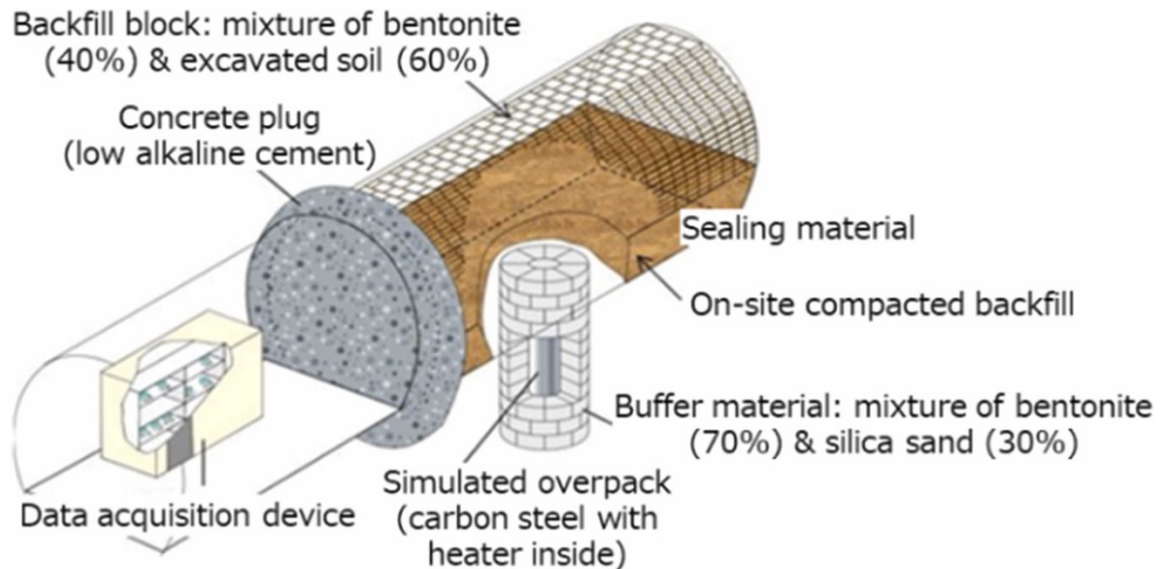


Figure 13. Schematic view of in situ EBS Experiment in the Horonobe URL in Japan, from<sup>43</sup>.

Six international research teams participated in Task D using a variety of computer codes, TH and THM formulations, and constitutive laws. Some joint lessons learned are briefly summarized below.

- Starting with comparative modeling of the laboratory tests before moving to simulations of the *in-situ* field test turned out to be successful in that it allowed reasonable prediction of the THM processes observed in the EBS Experiment.
- The temperature distribution in the engineered barrier was simulated well by all research teams. Reasonable agreement between the simulated results and the experimental data was also observed for water content, saturation, and pore pressure in the outer part of the buffer material, where the hydraulic behavior was measured with a psychrometer (Figure 14).
- Prediction results for mechanical behavior of the bentonite buffer differed depending on the choice of constitutive THM models. 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 was applied, adding an equation for considering swelling displacement improved the agreement with the measured deformation.
- Three-dimensional(3D) simulations of the EBS experiment were difficult to conduct for some teams due to the computational demand. Therefore, some research teams used two-dimensional(2D) axisymmetric or plane strain models instead. Such simplified 2D representations of the system were shown to be adequate but required careful assumptions to produce output that is directly comparable to the data.

More information on the collaborative research work conducted in the EBS Experiment is provided in the synthesis paper by Sugita et al.<sup>43</sup>. Detailed results from individual modeling groups simulating the laboratory and field experiments can be found in two additional papers<sup>44,45</sup>.

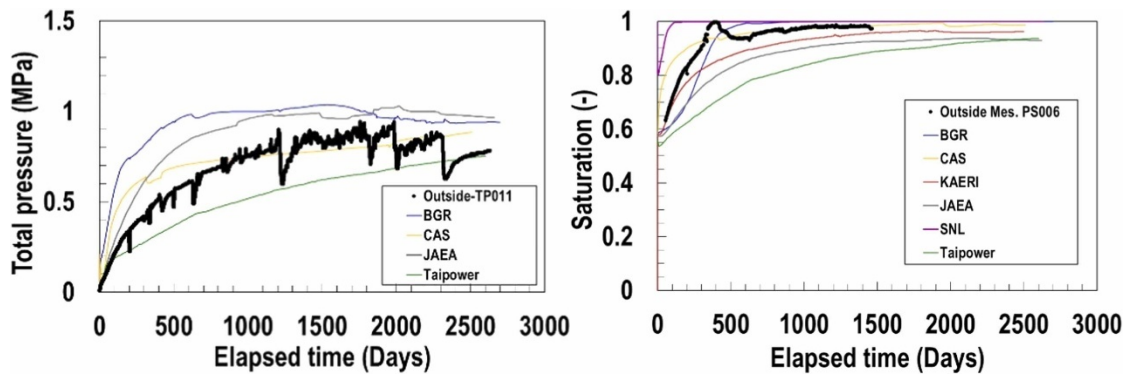


Figure 14. Example comparison of experimental observations versus model results for total pressure (left) and water saturation (right) measured in the outer part of the buffer material, from<sup>43</sup>.

### 2.3 Safety Assessment Models and Methods

Whereas previous phases had almost exclusively focused on complex physics-based models for complex coupled processes, DECOVALEX-2023 broadened this scope and started joint modeling work to build confidence in the system-level performance assessments (PA) and safety assessments (SA) of deep geologic repositories. Task F involved a staged comparison of the PA and SA frameworks, models and methods used by participating teams, focusing 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, for example radionuclide flux from one component of the system to another. Task F investigated two generic reference cases in parallel: a deep geologic repository in a fractured crystalline host rock (Task F1) and a deep geologic repository in a domal salt formation (Task F2). In both cases, the objective was to explore the contribution of modeling choices to uncertainty in PA and SA model outputs.

#### Task F1: Comparing Modelling Approaches for a Generic Nuclear Waste Repository in Crystalline Rock

Task F1 moved from a benchmarking phase involving flow and transport in simplified fracture geometries to comparative modeling of the large-scale reference case for a mined repository in fractured crystalline rock. The eight research teams in Task F1 used alternative modeling approaches, including explicit discrete fracture network (DFN) models, DFN upscaling to an equivalent continuous porous medium (ECPM), and a combination of both methods. Transport mechanisms were modeled using either the advection-dispersion equation or particle tracking.

A first synthesis paper by Mariner et al.<sup>46</sup> describes the benchmarks developed for Task F1 and discusses useful methods for analyzing the results. The benchmarks simulate flow and transport through a 1 km<sup>3</sup> block of fractured rock. The first involves migration of a short pulse of tracer through a simple network of four intersecting fractures. The second adds 1089 stochastically generated smaller fractures. The third changes the pulse to a continuous point source. Evaluation of model performance relied on moment analysis and comparison of the results of different models. Results demonstrate strong agreement among the models in breakthrough behavior up to the 75th percentile. Significant deviations in first moments and well-clustered outputs led to the identification of inaccuracies in several models. Such findings exemplify the benefit of exercising these benchmarks and using the presented methods to test DFN flow and transport models.

In a second synthesis paper for Task F1, Leone et al.<sup>47</sup> describe the collaborative modeling results for radionuclide transport from a mined repository in fractured crystalline rock. The generic modeling case was designed as a simplified version of a safety assessment, neglecting waste package performance and focusing on the transport of two conservative tracers from a waste canister deposition hole to the surface (Figure 15). Different quantities of interest were compared, such the amount of tracer remaining in the repository or the 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. For the models with a comparable representation of repository design, there were still some differences in model results. The main differences between these models were in the choices of how to represent the fracture network and simulate transport of the two tracers. The differences in the results indicate the sizeable effects of model form uncertainty and demonstrate the utility of comparing a range of approaches to PA and SA (Figure 16).

The synthesis papers<sup>46,47</sup> are complemented by two papers highlighting the model developments and results from two individual modeling groups: The first<sup>48</sup> describes employing two particle tracking methods, velocity interpolation and cell-jump, to simulate tracer transport for the benchmark cases, while the second<sup>49</sup> uses the upscaled ECPM method to model the full reference case of a repository in fractured crystalline rock.

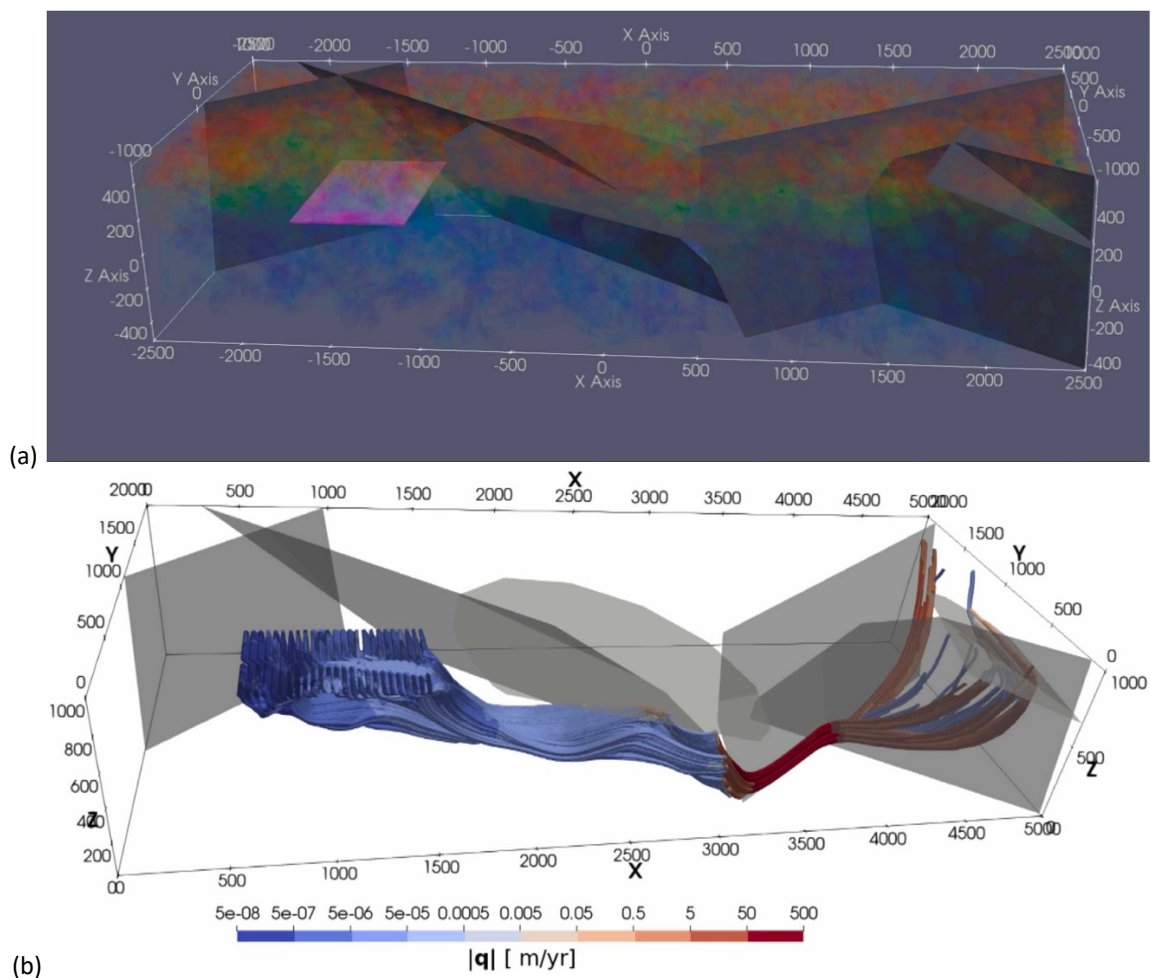


Figure 2. (a) Transparent view of model domain with deterministic and stochastic fractures. Colors represent different fracture families with repository location in magenta. (b) Illustration of streamlines starting at canister positions for the simulated stationary flow in the fracture network, based on results from one of the participating teams. Flow was simulated assuming a hydraulic pressure gradient from left (high point) to right (low point) imposed via Dirichlet boundary conditions at the top surface. Surface elevation decreases 20 m over a distance of 2 km; it was that assumed the hydraulic pressure mimics the topography. From<sup>47</sup>.

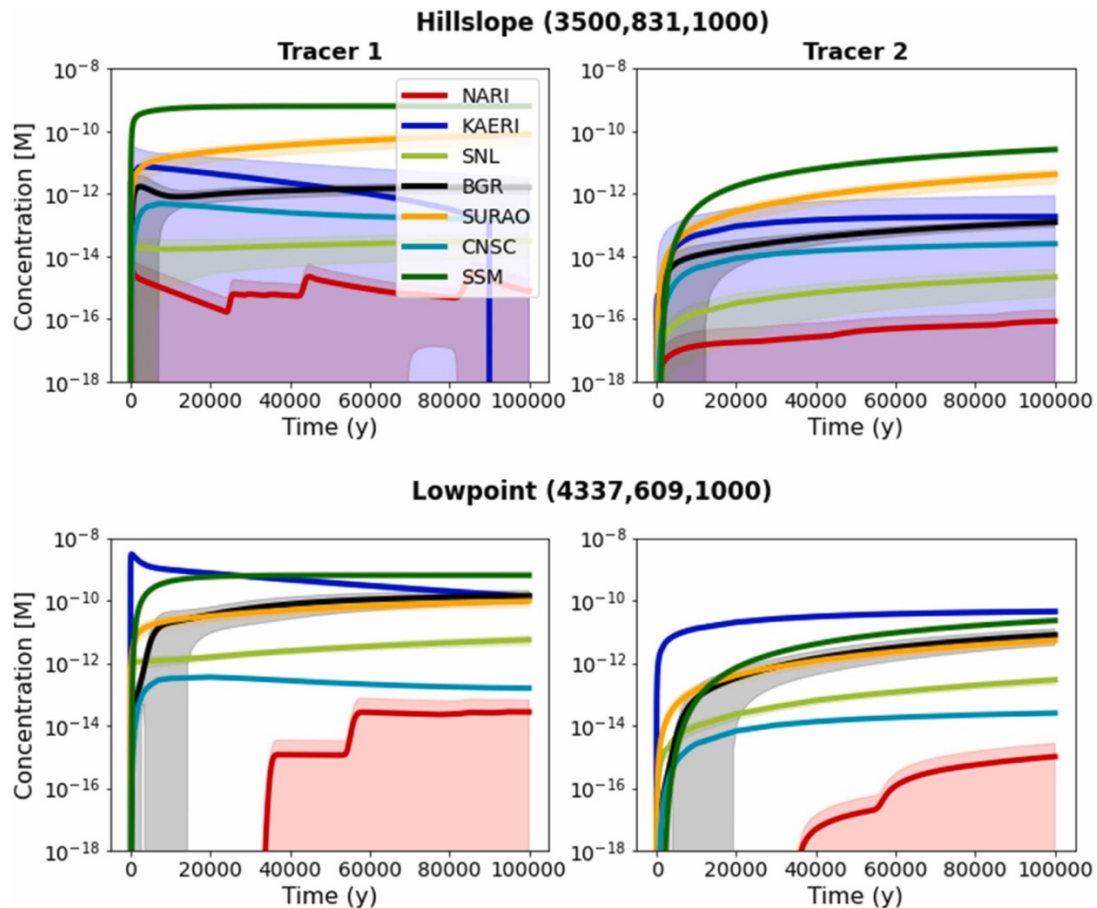


Figure 16. Comparison of transport simulations between participating teams. Means and 95 % confidence intervals of the means, for concentration [M] at the observation point on the hillslope (top row) at coordinate (3500,831,1000) and the low point (bottom row) at coordinate (4337,609,1000) for Tracer 1 (left column) and Tracer 2 (right column) for each team. SSM includes only one realization. From<sup>47</sup>.

#### Task F2: Comparing Modelling Approaches for a Generic Nuclear Waste Repository in Salt

This reference scenario for Task F2, developed collaboratively by the task participants<sup>50</sup>, contains realistic data for many of the key features, events, and processes for disposal in a domal salt repository (Figure 17). The base case centers on a disturbed (or alternative) scenario that has pessimistic assumptions about important engineered barriers: First, the shaft seals fail 1000 years after repository closure, allowing an influx of brine from overlying aquifers down the shafts and into the repository. Second, the vitrified glass begins dissolving at the start of the simulation and the spent nuclear fuel (SNF) containers simultaneously fail at 500 years. As described in the synthesis paper of LaForce et al.<sup>50</sup>, the five participating modeling teams used their own conceptual and computational models to simulate the evolution of the repository system. The interpretation of the simulation results was focused on performance measures indicative of the ability of the disposal system to isolate radionuclides in the subsurface through containment and retardation. Performance measures included those related to the overall performance of the repository system and those related to the performance of individual components of the engineered or natural system, such as resaturation and radionuclide transport from one component of the system to another.

All teams involved in Task F2 made simplifying assumptions in their models relative to the conceptual model in the task specification<sup>50</sup>. This resulted in a wide range of model dimensionality, ranging from compartmentalized network models to full 3D representations of the salt formation and repository (Figure 18). Another common simplification related to the choice of the salt creep-closure model. Despite differences in the modelling strategies, all models indicated 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 suggested that little of the disposed radionuclides will migrate beyond the repository

seal over the 100,000-year simulations (Figure 19). In general, the largest differences in model output occurred over the short term and in the near field of the repository. Disparities between the models were attributed to differing simplifications from the conceptual model.

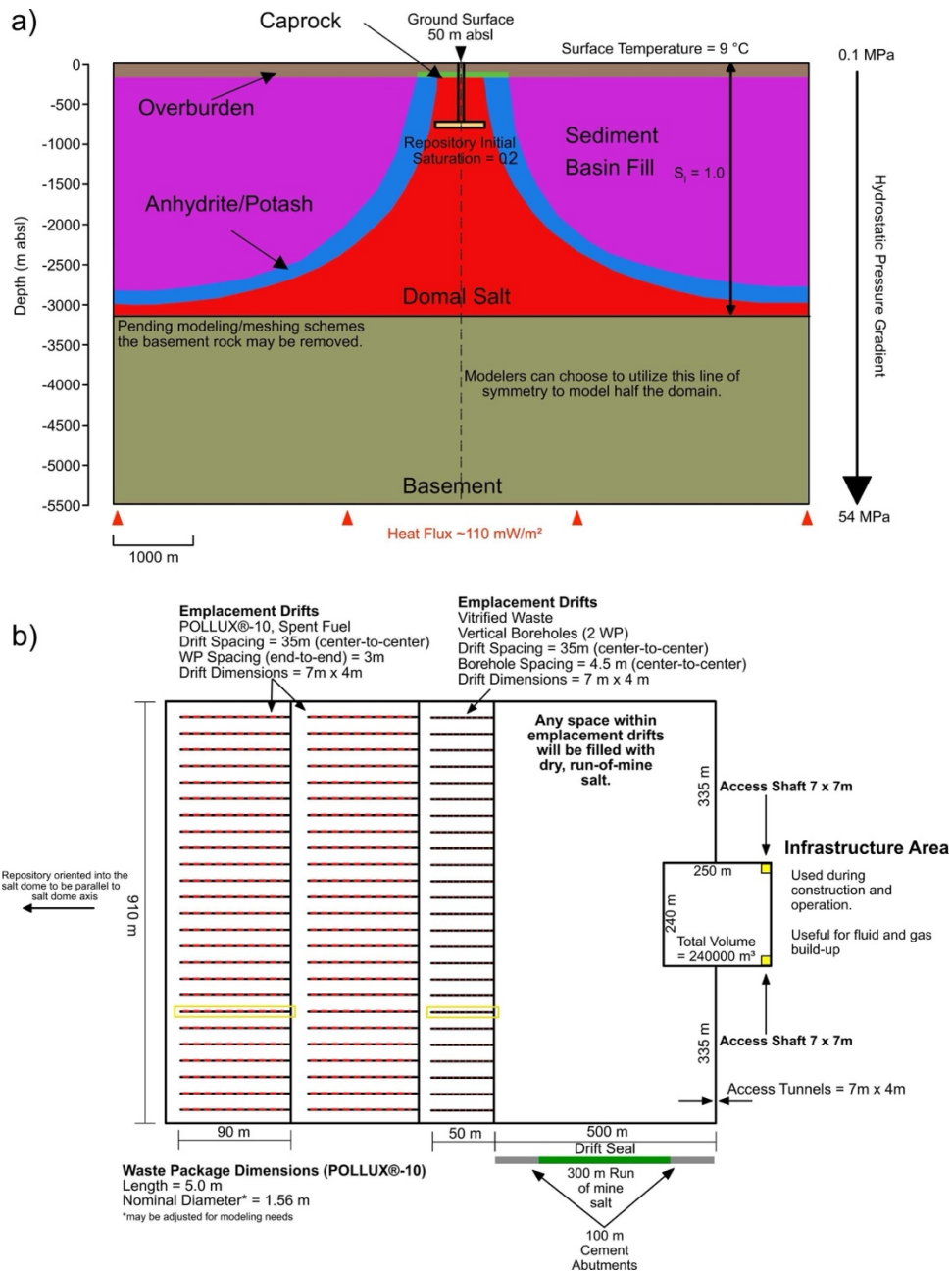


Figure 3. (a) Geological cross-section with model units for the generic salt reference case. The repository location and initial model conditions are shown. (b) Schematic of the waste repository in the generic salt dome. Quantities of interest (QOI) to be compared are in the highlighted areas. The drift seal is shown in green, while the lower shafts and waste drifts are highlighted in yellow. From<sup>50</sup>.

Additional analysis for the domal salt reference case examined the consequences of employing different levels of abstractions when modelling the repository's geometry and implementing various features and processes<sup>51</sup>. The discussion focused on when simplifications can be appropriately applied and what consequences result from them. Furthermore, it was explored when and if a higher level of fidelity in geometry or physical processes is required. Bartol et al.<sup>52</sup> expanded on the reference case to identify commonalities and differences between the teams for specific changes in repository design. Based on the lessons learned from Task F2, another study conducted a preliminary safety assessment for a geological disposal facility in rock salt in the Netherlands, based on the Dutch disposal concept and waste inventory<sup>53</sup>.

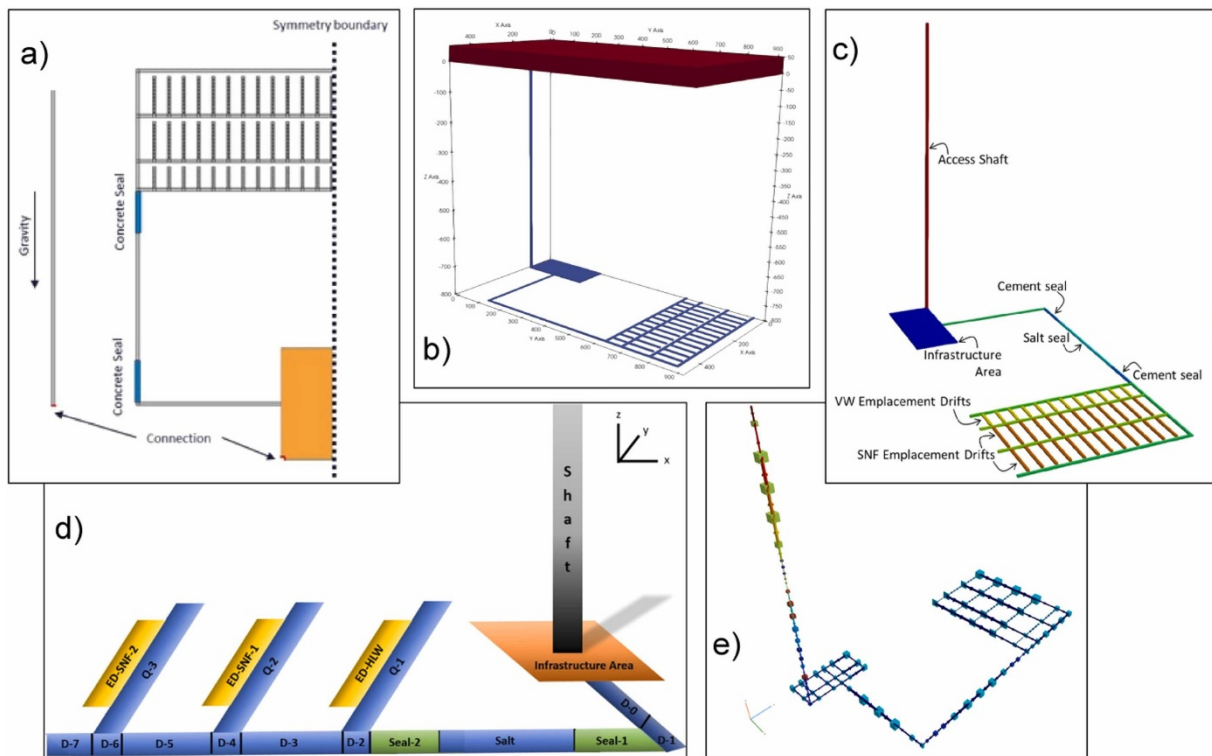


Figure 18. The different model layouts deployed by five teams participating in this performance assessment modeling task. From<sup>50</sup>.

### 3. Summary and Conclusion

As coordinators and guest editors of this Virtual Special Issue, we like to express our thanks to the funding organizations of the DECOVALEX-2023 initiative, to the task leads for designing the modeling challenges and coordinating the team’s efforts, to the research teams and authors of the papers for their scientific contributions, and to the editors of this journal. We hope that the summary presented above, and the in-depth research findings in the selected papers, provide an idea of the breadth and depth of cutting-edge research work carried out within the DECOVALEX-2023 initiative. Comparison of model results with other international modeling groups, using their own simulation tools and conceptual understanding, enhances confidence in the robustness of predictive models used for performance assessment. In addition, the possibility of linking model differences conceptual model choices provides valuable guidance into “best” modeling practices and understanding the effect of conceptual models on predictions. With this Virtual Special Issue, we also intend to convey to interested readers the value of the DECOVALEX philosophy of cooperation between international researchers of different disciplines using a range of different approaches. Such collaboration means frequent interactions, sharing of data and results, collectively generating new ideas and concepts, raising technical issues in joint communications, and performing critical reviews of each other’s work. The insight obtained in such integrated cooperative efforts would have been impossible if the teams had worked independently.

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