Brine Availability Test in Salt: International Collaborative Modeling in the DECOVALEX Project – 22164

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ABSTRACT

The Brine Availability Test in Salt (BATS) experiment is an ongoing phased heater experiment being conducted at the Waste Isolation Pilot Plant to study, in part, the origin and abundance of brine to sources of heat in bedded salt formations. The BATS experiment is one of several tasks in the international research and model comparison project known as the DEvelopment of COupled models and their VALidation against EXperiments (DECOVALEX). Each team participating in this DECOVALEX task has demonstrated accurate simulations for the prediction of the temperature distribution around a heat source in a salt formation as well as simulation of the brine migration to a single borehole in salt. These initial solutions to thermal (T) and hydrologic (H) equations have been combined with mechanical (M) equations that couple stress and strain to pressure and temperature into a fully-coupled THM simulation. THM simulations can predict the pressure pulse in salt formations exposed to heat by including the important process of thermal expansion of both rock salt and brine. Additional and more complex modeling benchmarks include simulations with multiple wells and multiphase simulations. Here we will present the progress of our uncoupled and coupled TH and THM simulations as well as insights we have gained into understanding the THM behavior of the EDZ and strategies for conceptual model development during benchmarking.

INTRODUCTION

The Department of Energy Office of Nuclear Energy (DOE-NE) disposal research and development program seeks to provide a sound technical basis for multiple viable disposal options, increase confidence in the robustness of generic disposal concepts, and develop science and engineering tools needed to support disposal concept implementation. As part of this program Los Alamos, Sandia and Lawrence Berkeley National Laboratories (LANL, SNL, and LBNL) are involved in the Brine Availability Test in Salt (BATS) which was first proposed by [1]. BATS is an ongoing heated borehole experiment being conducted in the underground at the Waste Isolation Pilot Plant (WIPP). The goal of this experiment is to reduce the uncertainty associated with spent nuclear fuel disposition in geologic salt formations. The BATS experiments are designed to accomplish this by increasing our understanding of brine migration in salt, assessing damaged zones from mining and drilling, simulating a post-closure environment, confirming salt properties, and providing data for model validation.

Part of LANL, SNL, and LBNL's model validation occurs through participation in the international research and model comparison project known as DECOVALEX, which brings together teams from around the world to advance our understanding and ability to simulate relevant coupled thermalhydrological-mechanical-chemical (THMC) systems. Currently DECOVALEX is in its 8th 4-year iteration which runs from 2020 to 2023 and includes 17 international organizations working on 7 different modeling tasks. For this iteration, the BATS experiment was chosen as Task E.

The objective of Task E is to use historical experiments and the current BATS experiment to develop THMC simulations which capture the necessary physical processes to predict brine availability in bedded salt formations. The THMC processes are highly coupled in salt [2] and some processes or the degree of coupling are uncommon in other materials. For example, the thermal conductivity of salt is high and displays a strong temperature dependence. Thermal pressurization is another example, due to the very low hydraulic diffusivity of salt. This pressure may drive some brine away from sources of heat. Salt also creeps in response to deviatoric stress, this creep rate is also pressure and temperature dependent. In addition, the heating of brine may drive evaporation and condensation of brine/water which can drive dissolution and precipitation of the rock salt formation and crushed salt backfill [3-5]. These attributes, such as the high thermal conductivity and salt creep are considered beneficial to long-term barrier performance. Other aspects, such as the thermal pressurizations effect on brine availability to sources of heat are less understood and a focus of the BATS experiment.

Compounding the THMC coupled processes is the presence of an excavation damaged zone (EDZ) surrounding rooms and boreholes in salt. The EDZ is characterized as a partially saturated fractured zone with higher porosity and permeability than intact salt. The EDZ is surrounded by a larger excavation disturbed zone (EdZ) which has less damage than the EDZ, but still has a perturbed state compared to the far field. The porosity in the EDZ and EdZ ranges but may be 10x that of the intact salt while permeability can increase by 6 orders of magnitude [6]. The evolution of the EDZ and EdZ through time and space (Figure 1) is a significant complication which likely has a large control on brine availability. The EdZ extent is controlled by the radius of the excavation and does not affect the far field barrier performance. However, in the early phases of waste storage, before creep closure occurs, the EDZ and EdZ likely play an important role on brine availability to waste packages and thus encourage the degradation of waste packages.

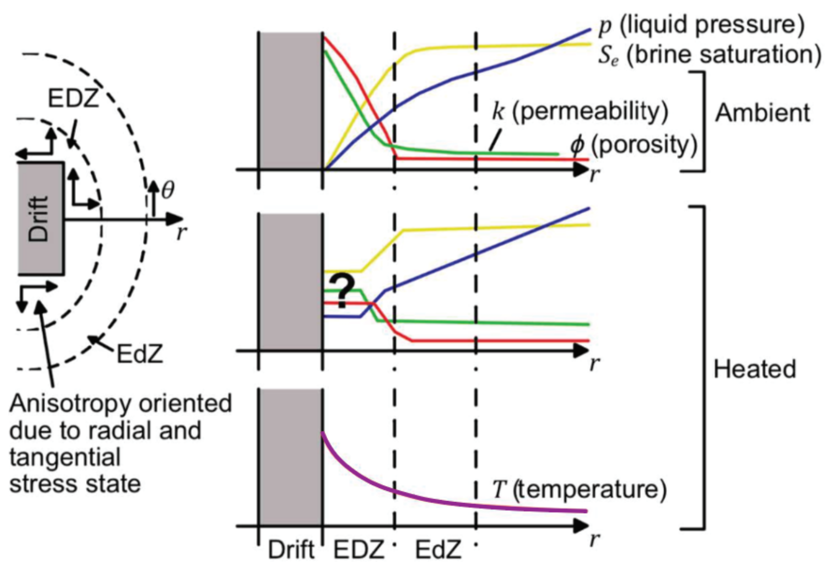


Figure 1: Evolution of properties in the EDZ and EdZ besides a drift [7]. In the ambient case the trends of liquid pressure, brine saturation, permeability, and porosity in the EDZ are somewhat understood. In the heated case only the temperature profile within the EDZ is well understood.

Kristopher Kuhlman (Sandia) is the Task E lead, and five teams representing four nations and seven institutions are participating in DECOVALEX Task E. The list of teams includes: the German Federal Institute for Geoscience and Natural Resources (BGR; Bundesanstalt für Geowissenschaften und Rohstoffe); the Central Organization for Radioactive Waste in the Netherlands (COVRA; Centrale Organisatie Voor Radioactief Afval); the United States Department of Energy (DOE); Global Research for Safety in Germany (GRS; Gesellschaft für Anlagen- und Reaktorsicherheit); and Quintessa, a scientific consulting firm based in the United Kingdom working with Radioactive Waste Management (RWM), a subsidiary of the UK Nuclear Decommissioning Authority.

Each institution is using a different modeling tool (Table 1). OpenGeoSys is an open source multi-physics platform for the simulation of THMC processes in porous and fractured media primarily developed out of the Helmholtz Centre for Environmental Research (UFZ, Germany). COMSOL is a general-purpose commercial finite element multiphysics simulation package, which allows for the coupling of partial differential equations through a graphical user interface and is suitable for many applications. CODE_BRIGHT is a THM finite element simulator for Coupled Deformation, BRIne, Gas and Heat Transport problems and was initially developed with a focus on saline media. FEHM (Finite Element Heat and Mass Transfer Code) is an open source finite volume THMC simulator that was developed at Los Alamos National Lab. FEHM has had many functions added specifically for simulating salt repositories. TOUGH-FLAC is an open source THMC simulator developed at LBNL linking the TOUGH integrated finite differences family of a multiphase fluid and heat transport codes with the commercial finite difference FLAC3D geomechanical simulator and has salt specific functions added. PFLOTRAN is a community-developed massively parallel open source finite volume THMC simulator (pflotran.org). Finally, QPAC is a finite volume multiphysics simulator developed by Quintessa.

TABLE 1: Summary of Task E teams and their modeling tools. The DOE team is composed of LANL, LBNL, and SNL.

Team	Modeling Tool	Type
BGR	OpenGeoSys	Finite Element Multiphysics
COVRA	COMSOL	Finite Element Multiphysics
GRS	CODE_BRIGHT	Finite Element THM
DOE: LANL/LBNL/SNL	FEHM – LANL TOUGH – LBNL/SNL PFLOTRAN - SNL	Finite Volume TH(M)C
RWM/Quintessa	QPAC	Finite Volume Multiphysics

DECOVALEX METHODOLGY

The Task E modeling tasks increase in complexity, beginning with uncoupled heat and single-phase brine transport and ending with coupled two-phase THMC simulations. This allows teams to validate different aspects of their modeling tools and conceptual models before tackling coupled processes where the cause of differences in simulation output between the teams may be harder to ascertain.

There are two main differences in each teams' modeling activities: both the implementation of the modeling tools and the conceptual models used by each team. It is not the goal of DECOVALEX to benchmark each code against one another, instead the teams attempt to borrow the best points of each other's conceptual models to develop a better understanding of modeling coupled processes in salt. During some steps benchmarking against one another has been attempted by settling on a single model with the same mesh design, initial conditions, and boundary conditions. However, despite these efforts, differences still arise between the models. For example, the implementation of boundary conditions may vary across the different simulation tools requiring modifications to the conceptual models.

The DECOVALEX project is organized into four "steps" beginning with step 0 [7]. Each step is broken down into smaller subtasks based on benchmarks or simpler comparisons. Step 0 is focused on modeling uncoupled single process H and T benchmarks while step 1 is focused on modeling TH, THM, and two phase (H^2) benchmarks. Step 0 was conducted from April 2020 through April 2021 and includes a benchmark from historical brine inflow experiments conducted by [8] as well as the observed temperature response to phase 1 of the BATS experiments. Step 1 began in November 2020 and includes a TH and THM benchmark to the analytical solution of brine production to a heated borehole presented by [9], and a two phase flow benchmark. The final task in Step 1 is a THM simulation of the Phase 1A BATS experiment and has not been completed yet.

Step 0: Small-Scale Brine Inflow Experiment from Finley et al., 1992

The experiments by [8] were designed to monitor brine inflow into freshly drilled boreholes at WIPP. A total of 17 boreholes were completed, however for Task E the teams focused on observations from 5 boreholes (L4B01; DBT10, DBT11, DBT12, and DBT13; Figure 2). L4B01 is a 10-cm diameter nearly horizontal borehole completed in the argillaceous halite of Map Unit 0 (MU-0) in Room L4. DBT10, 11, 12, and 13 are vertical boreholes drilled into the floor of Room D approximately 3.5 years after the room was excavated. The completion of L4B01 entirely within MU-0 makes it the simplest modeling case while the chosen DBT boreholes span various map units, including a disseminated clay seam (Clay F, Figure 2).

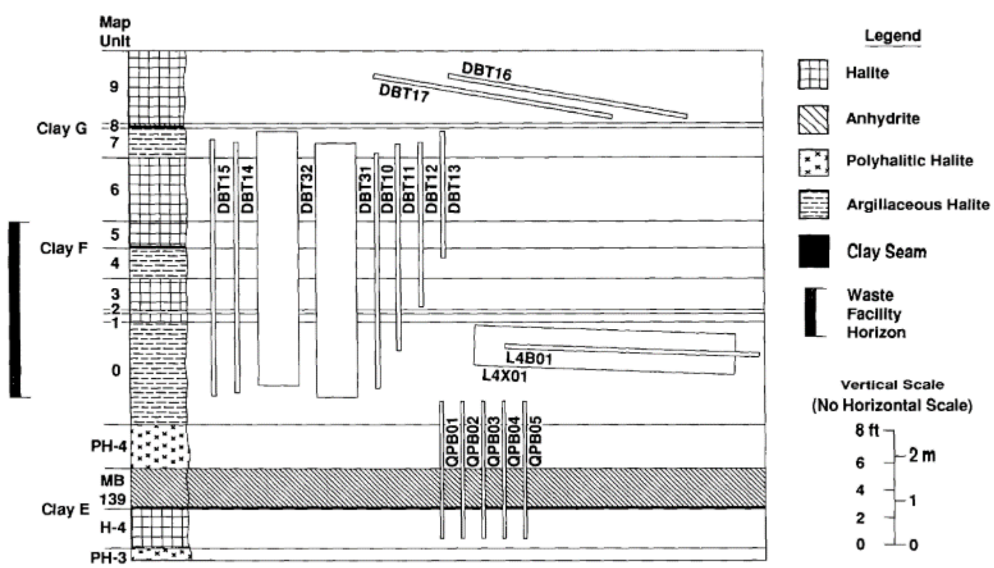


Figure 2: Location of boreholes with respect to lithologic units at WIPP. Small-Scale Brine Inflow Experiment from Finley et al., 1992.

Modeling of L4B01 is entirely contained in MU-0 making it the simplest of the models. Each team constructed their models using 1D or 2D radially symmetric geometries (Figure 3). LANL and

RWM/Quintessa included higher permeabilities meant to simulate an EDZ around the borehole while LBNL and COVRA neglected it. LANL and LBNL conducted multiphase flow simulations and LANL included the development of a pressure and saturation profile based on the mining of the drift and the drilling of the borehole [10] Despite these conceptual model differences, the results of each team were in relatively close agreement with each other and the observations (Figure 4). Given the simple nature of this problem the experimental data can be fit with a variety of model properties and boundary conditions.

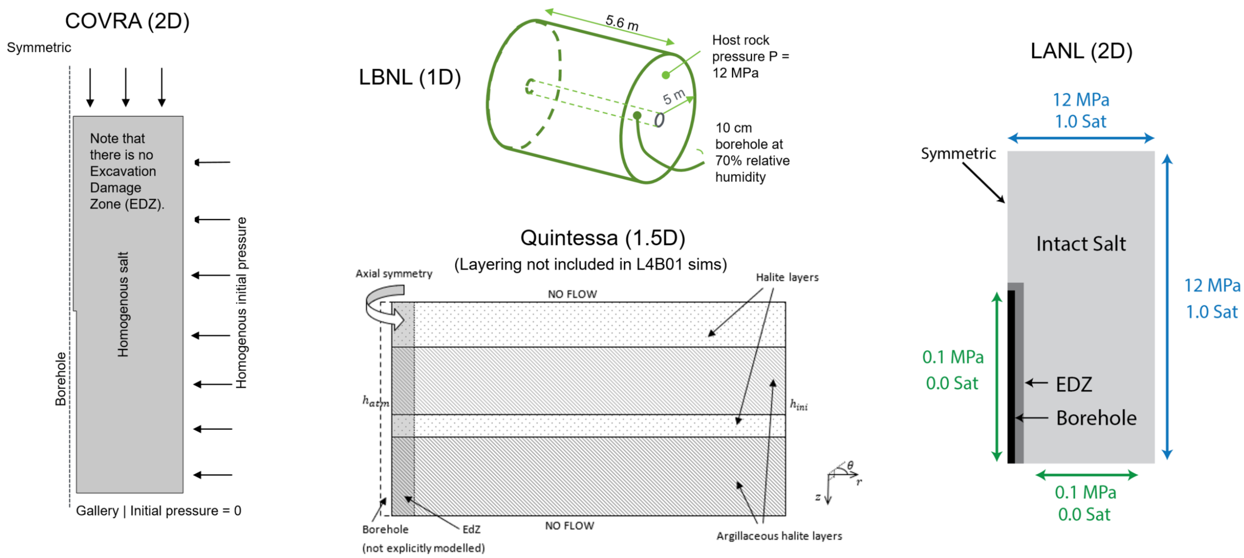


Figure 3: Conceptual model for L4B01. RWM/Quintessa model is 2D however there is no vertical connection between the nodes in the mesh and is therefore described as 1.5D. During the L4B01 simulations RWM/Quintessa used a single homogeneous lithology, not layered.

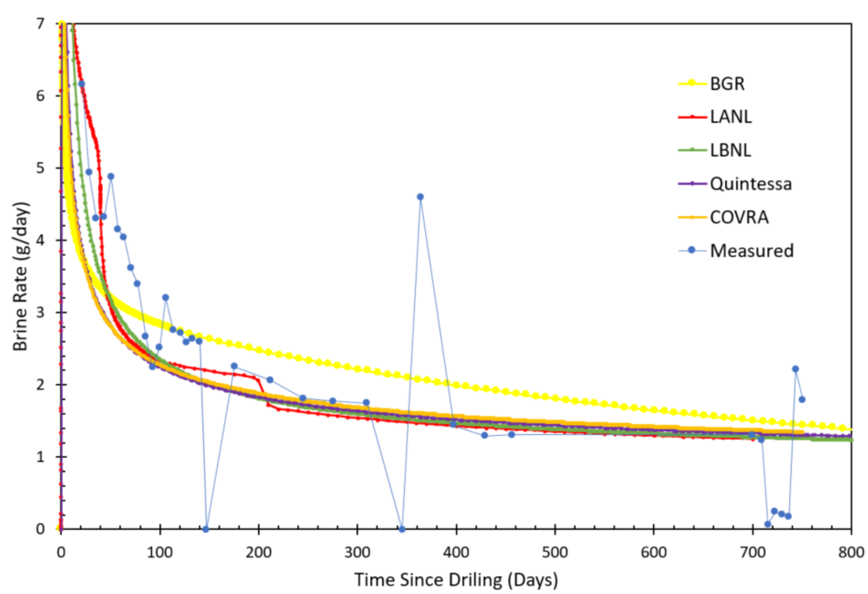


Figure 4: Brine inflow rates through time for horizontal borehole L4B01.

The Room D borehole benchmarking experiment is more complex due to the lithologic heterogeneity and the influence of multiple nearby wells. Each team was free to develop their own conceptual model of the experiment (Figure 5). Some models included the complete lithologic heterogeneity while others approximated the lithology with only a few units. Likewise, some models included boundary conditions meant to simulate multiple neighboring wells while others simplified to only one well. Despite these differences there was good agreement between each modeling team. Table 2 includes a summary of the different characteristics of each of the conceptual models shown in Figure 5.

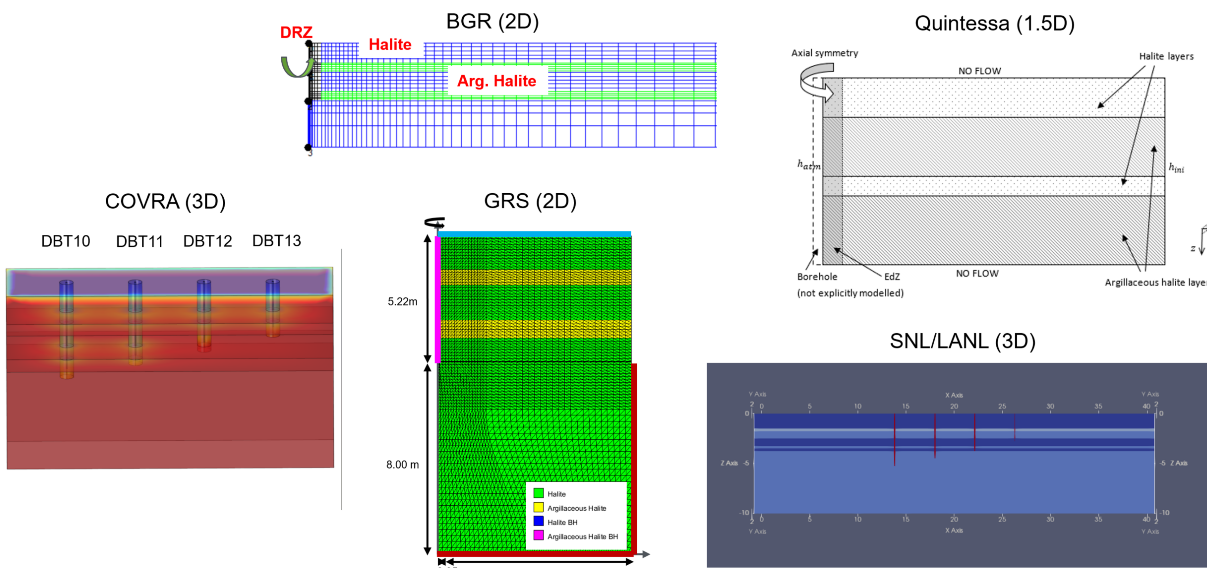


Figure 5: Conceptual Models of the Room D boreholes.

TABLE 2: Modeling properties used by each team for Room D benchmarking.

Team	Dimension	Borehole EDZ?	Drift EDZ?	Lithologic Variation?	Length (m)	Far Field Pressure (MPa)	Permeability (k)
BGR	2D	Y	N	Y	80	10	layers
COVRA	2D (+ 3D)	N	N	N	0.5–6	2–16	uniform
GRS	2D	N	N	Y	8	12	layers
DOE: LBNL	1D	N	N	N	5	12	uniform
DOE: SNL	3D	Y	Y	Y	5×10×40	12	layers
DOE: LANL	3D	Y	Y	Y	10×30×40	12	layers
RWM/ Quintessa	1.5 D	Y	N	Y	12	9–15	k(r)[a] in layers

Footnotes:
[a] Permeability is a function of the radial distance.

In general, each teams' brine inflow estimates to DBT10 and DBT11 are considered satisfactory (Figure 6). Due to the larger variation in conceptual models, a larger spread in results is expected than in the L4B01 benchmark. Only LANL and Sandia provided DBT12 and DBT13 results from their full 3D models. In these models some sacrifice of accuracy is necessary to best match other wells. This can be seen in Sandia's close simulation of the DBT10 and DBT11 experimental results but less accurate fit to DBT12 and DBT13. The LANL results are more accurate at DBT12 and DBT13 but less accurate at DBT10 and DBT11. This reflects the complicated interactions between boreholes completed near each other in bedded salt formations as well as the heterogeneity of the mapped units at WIPP. At approximately 800 days of drilling the flow rate appears to increase. The authors state that while there were no known experimental changes it is plausible that the development of excavation induced fracturing at this time caused both the erratic and increasing inflow rates.

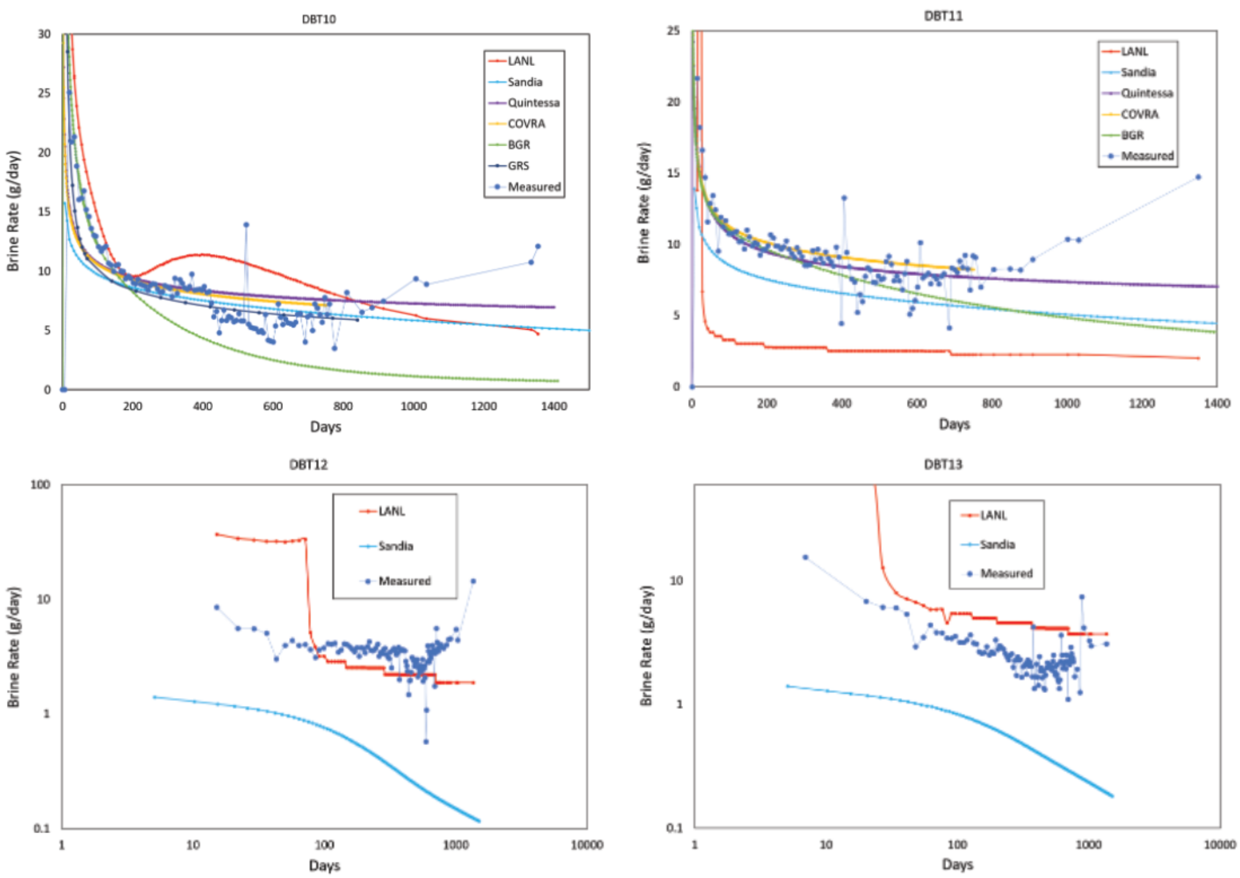


Figure 6: Brine inflow rate through time in simulations of vertical boreholes DBT10 (top left), DBT11 (top right), DBT12 (bottom left), and DBT13 (bottom right).

Step 0: BATS Phase 1 Temperature Response

The BATS experiment is a series of ongoing heated borehole experiments conducted underground at WIPP. The as-built experimental setup includes the drilling and instrumentation of two borehole arrays [11]. One array includes a heated borehole while the second array serves as an unheated control. Each array includes a central borehole (HP) with a heater (for the heated array only) and a packer as well as dry N_2 gas circulation to remove brine (Figure 7). Surrounding the central borehole are boreholes for temperature sensors only (T), acoustic emissions (AE), a cement seal (SL), tracer injection (D), electrical resistivity tomography (E), fiber optic monitoring (F), and liquid brine sampling (SM). A diagram of the heating apparatus in the central borehole of the heated array is provided in Figure 8.

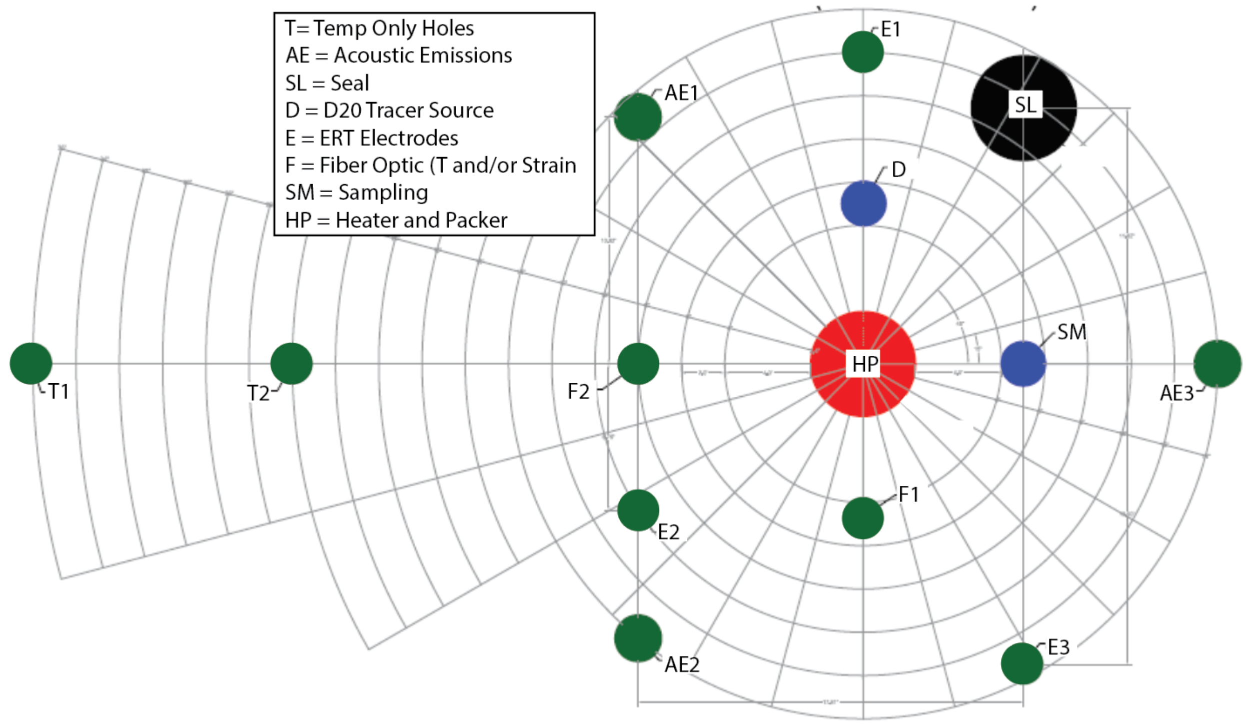


Figure 7. Borehole layout plan for each BATS test array (heated and unheated).

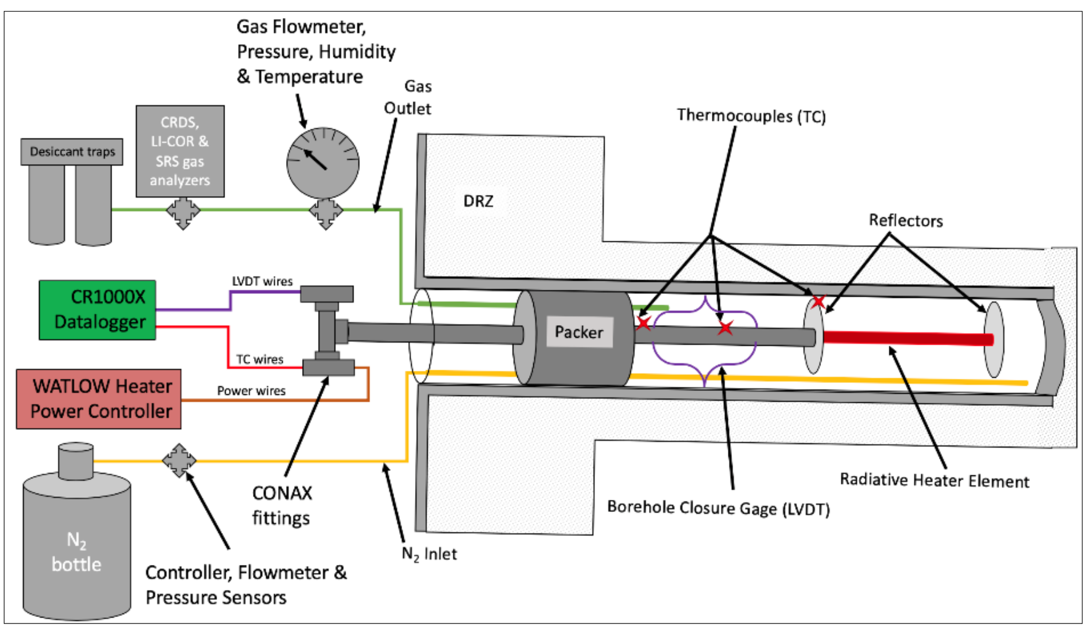


Figure 8. Conceptual wiring and plumbing diagram for the heated HP borehole.

The water inflow was not part of this benchmark and instead each team was asked to investigate the problem as a heat conduction problem in salt. Each of the conceptual models employed by the different teams is shown in Figure 9.

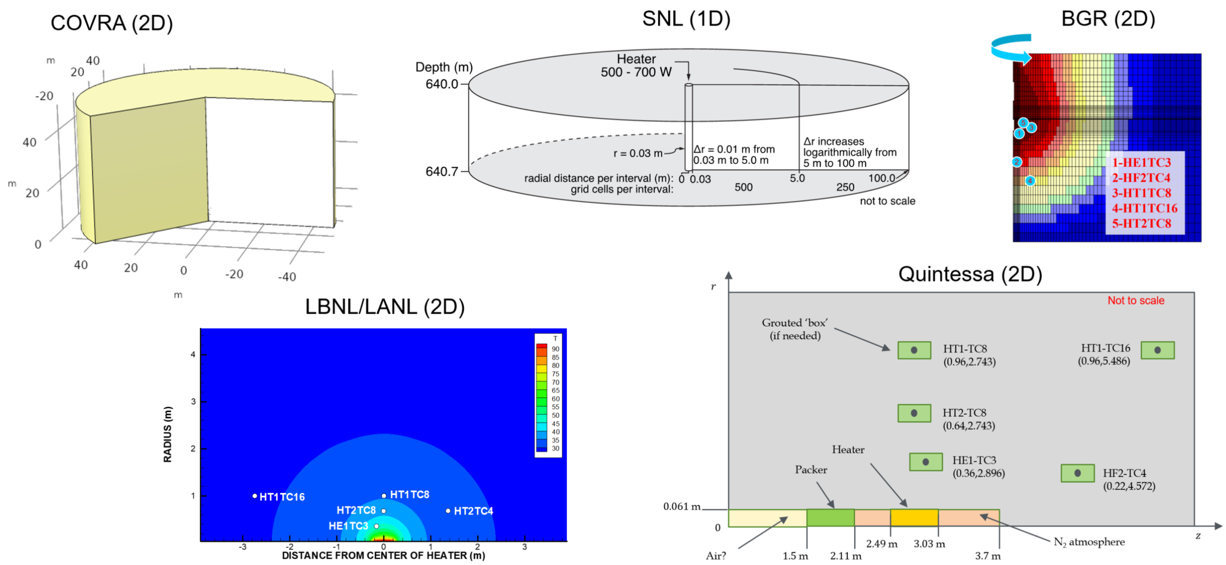


Figure 9. Conceptual models of each team's BATS Phase 1 thermal benchmark. LBNL and LANL developed two different simulations using the same conceptual model.

Each model varied in terms of the depth into the domain for the background temperature boundary condition, whether the thermal conductivity was a function of temperature, whether liquid was present (single phase or multiphase flow), and if a borehole or drift EDZ was present. Table 3 summarizes each teams' conceptual model and Figure 10 shows the results of each teams' simulations. The temperature was accurately modeled and each teams' simulated results compare well to each other. An important finding from this benchmark was that to accurately simulate the temperature response, either the thermal conductivity needed to be increased or the heater output needed to be decreased. Rather than attempt to directly fit the data, RWM/Quintessa chose to test whether the measured temperature-dependent thermal conductivity and specific heat capacity of WIPP salt [12] could adequately reflect the observations. In addition, several teams noticed slight adjustments in temperature sensor locations allowed for much improved ability to reproduce the observed temperatures. For example, RWM/Quintessa estimates that the heater was 91% efficient but that a single thermocouple needed to be moved 3 cm to provide the most accurate result. LANL also reduced their heater efficiency to 85%, and COVRA noted a different temperature sensor than RWM/Quintessa as being possibly slightly out of position. Overall, the proposed temperature sensor movements, adjustments to the heater output, and changes to the thermal conductivity are physically realistic.

TABLE 3: Conceptual modeling properties used by each team for BATS Phase 1 thermal benchmarking.

Team	Dimension	Liquid Present?	Borehole EDZ?	Drift EDZ?	$k_T(T)$[a]?	Depth (m)
BGR	2D	Y	Y	N	N	80
COVRA	2D (+3D)	N	N	N	Y	50
DOE: LBNL	2D	Y	N	N	N	5
DOE: LANL	2D	Y	N	N	Y	5
DOE: SNL	1D	Y	Y	Y	N	100
RWM/Quintessa	2D	N	N	N	Y	10

Footnotes:
[a] Thermal conductivity as a function of temperature denoted by $k_T(T)$.

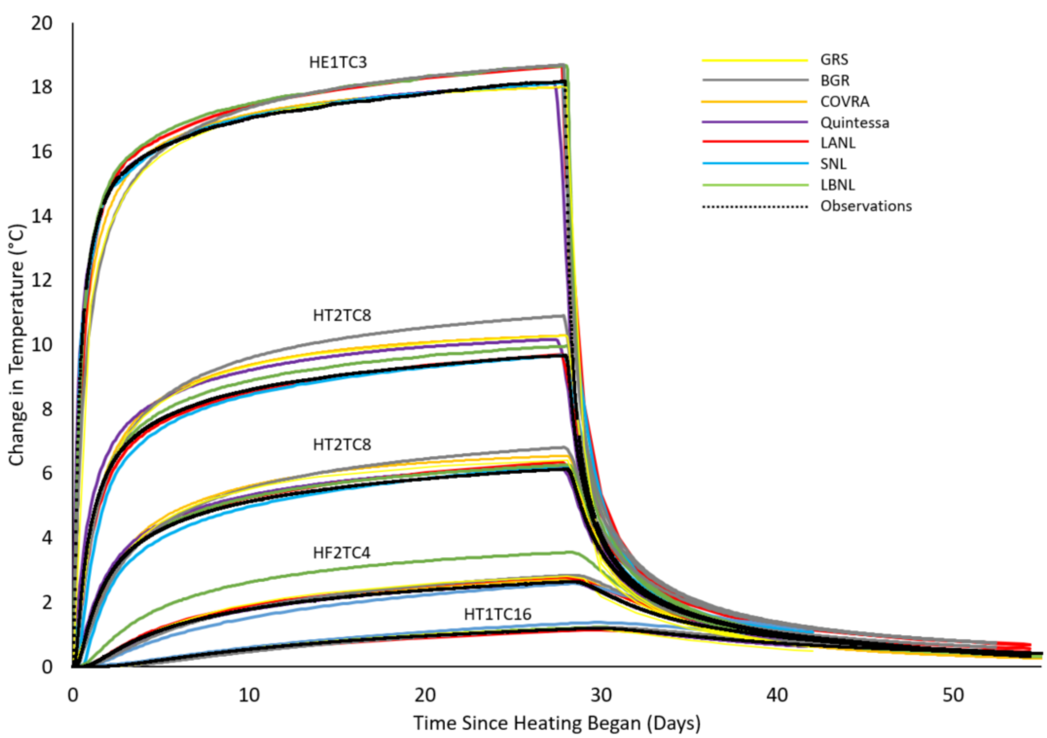


Figure 10: Temperature response vs simulation of the BATS Phase 1a experiment. Each thermocouple is designated first by an H or a U for the heated or unheated array, next by the borehole, and finally by the thermocouple number within the borehole. In order of increasing distance from the heater the thermocouples plotted are HT1TC16, HF2TC4, HT1TC8, HT2TC8, HE1TC3.

Step 1: Single-Phase Thermally-Driven Brine Production to a Heated Borehole [9]

While Step 0 focused on uncoupled H and T experiments, Step 1 begins the modeling of coupled processes (TH) with a benchmark by McTigue [9]. This benchmark investigates the thermal pressurization response of a heated borehole (without a regional pressure gradient). McTigue's analytical solution [9] was compared to each team's model using available salt properties [13]. In some cases, matching the analytical solution required disabling non-linear constative laws, such as temperature dependent fluid viscosity or thermal conductivity. Conceptual models varied considerably between teams (Figure 11).

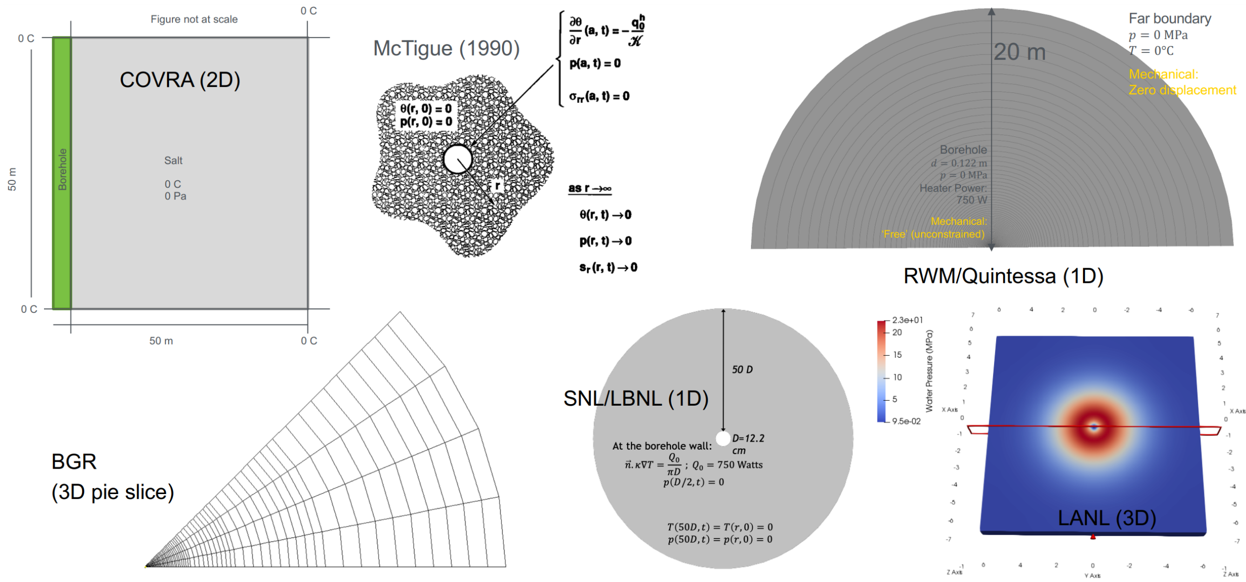


Figure 11: Conceptual models for the single-phase brine production to a heated borehole (McTigue benchmark [9]).

Some teams presented results based on TH simulations as well as THM simulations and investigated both a confined and an unconfined system (Table 4). The TH simulations include the thermal expansion of the brine but not the thermal expansion of the salt matrix, whereas the THM simulations are mechanically "confined" and include change in stress due to thermal expansion of the salt matrix. This is the first benchmark to include mechanical coupling and some teams investigated the problem using different simulators than previous benchmarks. LBNL utilized both COMSOL in addition to their usual TOUGH3 simulator to test the analytical solution provided by [9] SNL utilized TOUGH2 for the confined and unconfined system and PFLOTRAN only for the unconfined. The results of the unconfined and confined pressure response at 1 day and 1 week as well as the brine flux into the boreholes for each model is presented in Figures 12 and 13. The temperature results are not shown, because temperature modeling has already been successfully benchmarked, but the results were very closely aligned to the analytical solution.

TABLE 4: Conceptual modeling properties used by each team for the [9] benchmark.

Team	Dimension	TH/THM	R (m)
BGR	3D Slice	TH and THM	20
COVRA	2D	TH and THM	50 (1-9)
DOE: LANL	3D box	THM	6.1 – 8.6
DOE: SNL	1D	TH (PFLOTRAN/TOUGH2) THM (TOUGH2)	6.1
DOE: LBNL	1D	TH and THM	6.1
RWM/Quintessa	1D	TH and THM	20

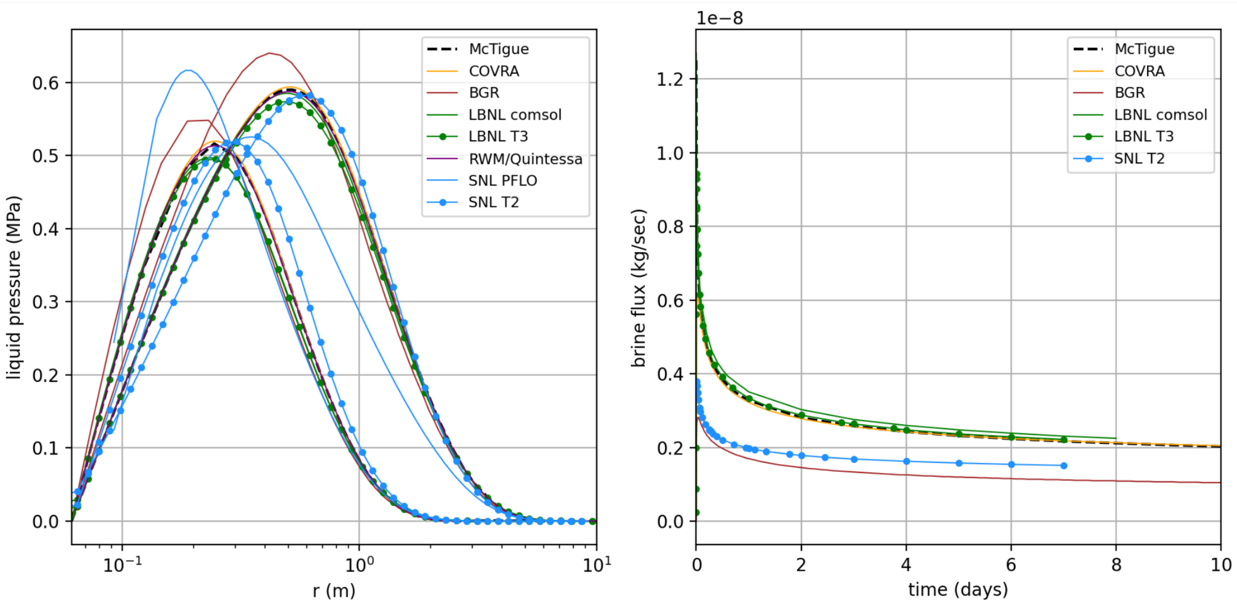
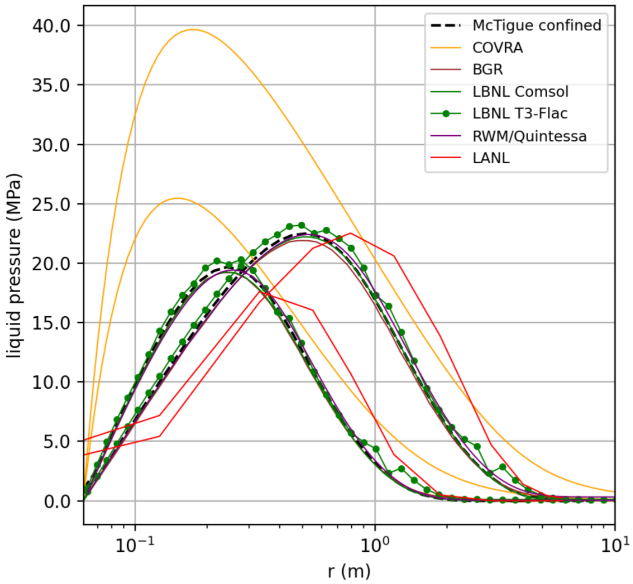


Figure 12: Simulations vs. unconfined analytical solution to the McTigue benchmark [9]. Smaller curve at 1 day and larger curve at 1 week. Liquid pressure and brine flux remain relatively low due to the lack of thermal expansion of the salt matrix.



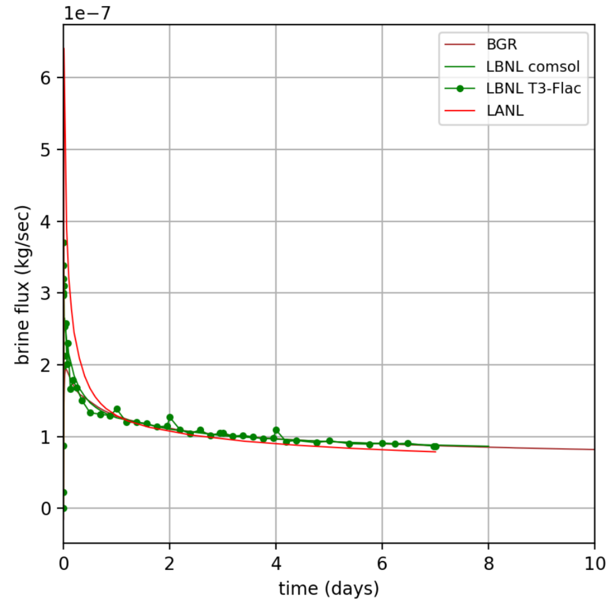


Figure 13: Simulation vs. confined analytical solution to the McTigue benchmark [9]. Smaller curve at 1 day and larger curve at 1 week. Liquid pressure and brine flux are much higher due to the mechanical confinement and expansion of the solid matrix.

The agreement between each team and the unconfined analytical pressure response (Figure 12) is considered satisfactory although some discrepancy from the analytical solution for water inflow is shown. For the analytical confined pressure response BGR, LBNL, and RWM/Quintessa appear very close to the analytical pressure response while LANL appears a little shifted and COVRA's pressures are too large (Figure 13). The water production values from each team are quite similar. This benchmark is important to understand the coupling of THM processes during the heating of borehole in a salt formation however, being single-phase, this benchmark assumes that the formation is completely saturated which may not be the case during the BATS experiments. This could have a significant effect on the pore pressure response to heating. McTigue discussed the confined THM solution but presented parameter values that result in models consistent with the unconfined TH solution [13]. This discrepancy illustrated that the analytical solution could be matched against either the confined or unconfined numerical approaches, by altering the effective thermal expansion coefficient (b' in that paper) by a factor of approximately 40.

Step 1: 1D Multiphase Flow

The final benchmark completed in Task E of DECOVALEX is a 1D axisymmetric simulation of multiphase flow to a newly excavated drift. Each team was asked to complete a simulation assuming a completely saturated 2.5 m EDZ surrounded by intact salt. The absolute permeability of the intact salt and EDZ are set to 10^{-21} m^2 and 10^{-17} m^2 respectively. Van Genuchten relative permeability curves used an m-value of 0.6, residual liquid saturation of 0.19, and entry pressures of 1.54 MPa for the intact salt and 0.0154 MPa for the EDZ. The porosity of the intact salt is set to 0.001 and the EDZ porosity is 0.01. The background pressure is 12 MPa and completely saturated and the drift is assigned atmospheric pressure. The initial saturation is set to 100% for the EDZ and intact salt. Due to the very prescriptive nature of this benchmark, all conceptual models developed are similar (Figure 14).

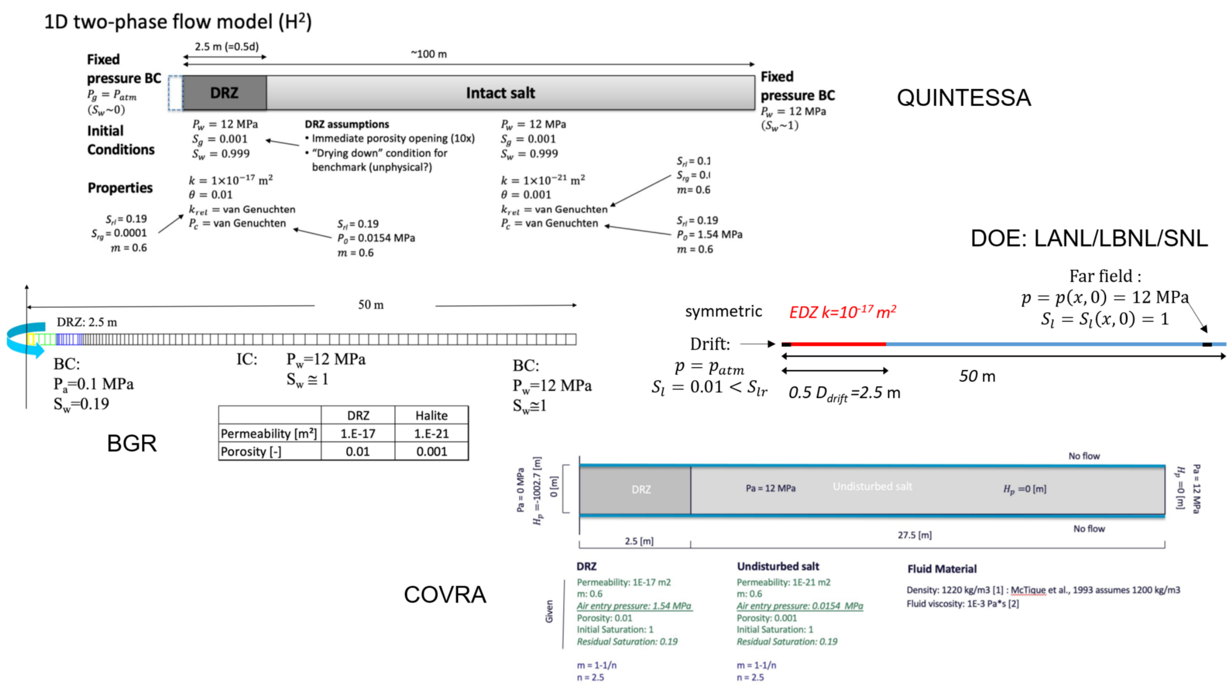


Figure 14: Conceptual models of 1D multiphase flow benchmark.

The results from each team are presented in Figure 15. The pressure results show a significant amount of variation at 1 hour, but by 1 month each team members' simulations are relatively similar with only small differences. The saturation profiles are very similar at one hour because the entire domain is mostly saturated, but by 10 years some differences are noted. All teams' simulations agree that even after 10 years the intact salt adjacent to the EDZ remains completely saturated. No team members agree on a single total brine production value however they all fall between approximately 25 and 225 kg. It is notable that even when relying upon a prescribed conceptual model each team produced a different estimate for the total brine flow. This provides some insight into the difficulties of benchmarking multiphase flow. If each team successfully implemented the benchmark, then these differences must be due to the different implementations within each modeling tool.

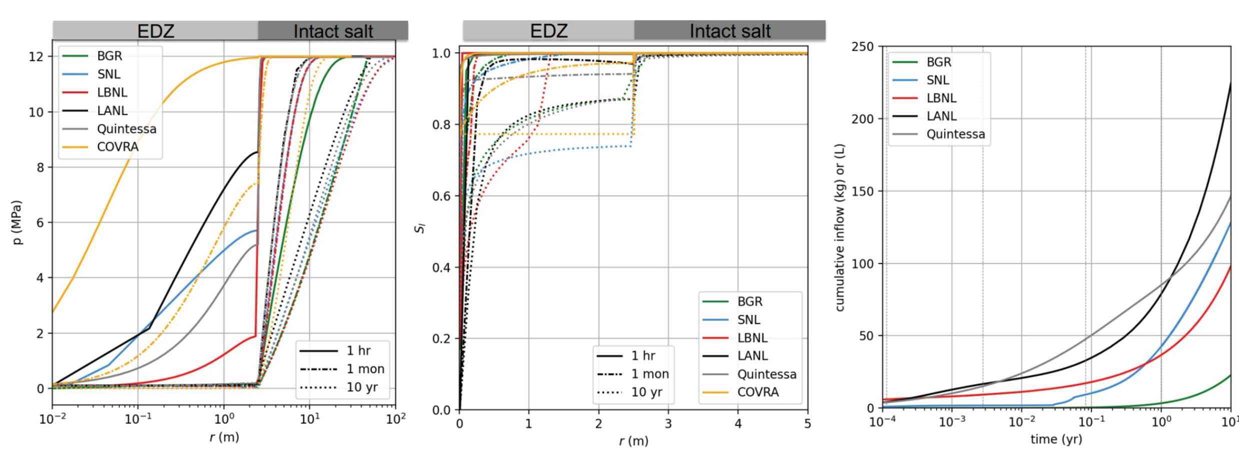


Figure 15: Results of the 1D multiphase flow benchmark. Results at 1 hour, 1 month, and 10 years for pressure (left) and saturation (middle). Total cumulative brine inflow to the drift (right).

While this benchmark assumed the EDZ was completely saturated, RWM/Quintessa illustrated clearly the difference in response due to initial conditions by running additional simulations with a 10% initial saturation in the EDZ. If the porosity is rapidly created due to geomechanical processes then it is likely to not remain fully saturated. Theoretically, if the EDZ has 10 times the porosity of the intact salt, as it does in the benchmark, then it would also be only 10% saturated if no water was allowed to move into or out of the EDZ when it formed. We call the fully saturated scenario a “drying down” simulation where the EDZ slowly dries out, versus a “wetting up” scenario where the EDZ is relatively unsaturated and becomes more saturated with time. Quintessa showed the “drying down” scenario, which is probably an inaccurate representation of reservoir conditions, creates 100x more brine inflow in 10 years than the “wetting up” scenario. This demonstrates the impact of the initial conditions on brine availability. The true inflow through a freshly created EDZ will most likely lie somewhere between the “drying down” and “wetting up” scenarios. Better understanding of the development of the EDZ is therefore important in determining likely flows to waste containers. The next step in Task E of DECOVALEX entails modeling the coupled BATS Phase 1A heat and brine production and may yield more insights into this process.

CONCLUSIONS

Close collaboration on experimental and numerical benchmarks has been extremely helpful for developing accurate THMC simulations for Task E in DECOVALEX. One of the most interesting aspects of this process is how each individual team approaches a particular problem by implementing different initial conditions and boundary conditions, even when modeling simpler benchmarks or uncoupled processes. The Room D benchmark which contained multiple wells has demonstrated the importance that lithologic heterogeneity and the interplay between each well has on brine production. This will be important to capture when modeling the BATS array which has many boreholes near one another. The McTigue benchmark [9] demonstrates the importance of being able to simulate the pore pressure effect that heating has on salt formations. This pore pressure forms a dam around sources of heat potentially leading to a decrease in brine availability and corrosion to waste canisters. However, it has been shown that this effect is reduced in a partially-saturated EDZ, since even a small amount of air makes the system much more compressible, and so the extent to which air can penetrate the intact salt beyond the EDZ will be an important controlling factor. Finally, the variety of results from the multiphase benchmark, despite its prescriptive nature, has shown that underlying differences in the codes can produce a wide range of saturation, liquid pressure, and brine production estimates. In addition, conceptual models developed as part of the multiphase work have challenged our initial modeling assumptions of a “drying down” scenario. The consensus conceptual model now favors the “wetting up” scenario which will have a significant impact on brine production simulations. By working collaboratively to understand how each team approaches and implements numerical representations of THMC simulations, all the members of the group learn from each other and expands the baseline understanding of coupled processes in the context of generic HLW repository science. Steps 2 and 3 of the DECOVALEX project will focus more on coupled processes in the BATS project [14]. We look forward to continuing this interesting collaboration and sharing the results with the scientific community.

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