Modeling and Field Test Planning Activities in Support of Disposal of Heat-Generating Waste in Salt

Fuel Cycle Research & Development

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APPENDIX E

FCT DOCUMENT COVER SHEET [1]

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This deliverable was prepared in accordance with Lawrence Berkeley National Laboratory
(Participant/National Laboratory Name)

QA program which meets the requirements of
☒ DOE Order 414.1 ☐ NQA-1-2000 ☐ Other

This Deliverable was subjected to:

☐ Technical Review

☐ Peer Review

Technical Review (TR)

Review Documentation Provided

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Peer Review (PR)

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ACRONYMS

EDZ	Excavation Disturbed Zone
EOS	Equation-of-State
LBNL	Lawrence Berkeley National Laboratory
REV	Representative Elementary Volume
THM	Thermal-Hydrological-Mechanical
THMC	Thermal-Hydrological-Mechanical-Chemical
TSDE	Thermal Simulation for Drift Emplacement

1. INTRODUCTION

In this report, we present FY2014 progress by Lawrence Berkeley National Laboratory (LBNL) related to modeling and field test planning activities in support of disposal of heat-generating waste in salt.

The modeling efforts in support of the field test planning conducted at LBNL leverage on recent developments of tools for modeling coupled thermal-hydrological-mechanical-chemical (THMC) processes in salt and their effect on brine migration at high temperatures as reported in the recent FY2014 milestone report entitled "*Modeling Coupled THMC Processes and Brine Migration in Salt at High Temperatures,*" FCRD-UFD-2014-000341 (Rutqvist et al., 2014). This work includes development related to, and implementation of, essential capabilities, as well as testing the model against relevant information and published experimental data related to the fate and transport of water. These are modeling capabilities that will be suitable for assisting in the design of field experiment, especially related to multiphase flow processes coupled with mechanical deformations, at high temperature. In this report, we first examine previous generic repository modeling results, focusing on the first 20 years to investigate the expected evolution of the different processes that could be monitored in a full-scale heater experiment, and then present new results from ongoing modeling of the Thermal Simulation for Drift Emplacement (TSDE) experiment, a heater experiment on the in-drift emplacement concept at the Asse Mine, Germany, and provide an update on the ongoing model developments for modeling brine migration. These activities are described in Sections 2, 3, and 4.

LBNL also supported field test planning activities via contributions to and technical review of framework documents and test plans, as well as participation in workshops associated with field test planning (Section 5).

2. RESULTS FROM GENERIC REPOSITORY MODELING

Based on the FY2014 model improvements, LBNL has completed a study of long-term THM behavior of a generic repository. Overall, the generic repository simulation results suggest that the excavation disturbed zone (EDZ) around an emplacement tunnel is healed within the first few years and that the backfill reconsolidates within the first two decades. Depending on the magnitude of the pore pressure relative to the minimum principal stress, damage-induced secondary permeability and fluid infiltration may occur at a larger temporal and spatial scale. Once damage processes are over, our predictions show that the initial tightness of the host rock is restored.

Though the generic repository modeling was conducted over a 100,000 year time frame, the results are also useful for studying the responses during the first few years, perhaps up to 10 or 20 years, to investigate THM responses that could be observed in a heater experiment. Figure 2-1 presents the model geometry and Figure 2-2 the evolution of some of the key parameters over the first 20 years. The initial heat load which decays marginally during the first few years was 1000 W per meter of drift. The host rock in this case is representative of the Asse Mine in Germany, which generally has a much lower porosity and water content than the host rock at WIPP. Nevertheless, from Figure 2-2 and other results discussed in Rutqvist et al. (2014), some observations can be made related to a potential heater experiment of an in-drift emplacement concept:

- A first thermal peak of about 200°C was reached on top of the waste package after about 1 year, after which the temperature within the backfill declines along with the reconsolidation of the backfill (Figure 2-2a).
- An excavation disturbed zone develops during the excavation and early time heating to a thickness about 1.4 m at the drift floor and 1 m at the sidewalls and roof with a peak dilatancy achieved after about 4 years (Rutqvist et al., 2014).
- Along with the temperature mediated salt creep of the host rock, the reconsolidation of the crushed salt takes place, though not uniform in space, due mainly to the shape of the drift and the position of the heat source (Figure 2-2b).
- Greater compaction occurs in the roof and floor areas, and lesser compaction in the sidewalls, and the backfill reconsolidation process takes between 6 and 20 years to complete (Figure 2-2b).
- The occurrence of healing is closely related to the backfill compaction, and after 7 years, dilatancy has decreased to its initial value, meaning that the host-rock tightness is restored (Rutqvist et al., 2014). .
- Within the first year, a slight desaturation of the host rock occurs adjacent to the drift wall, whereas moisture content increases up to 3.5% within the crushed salt backfill near the top of the drift (Figure 2-2c).
- Thermal pressurization and backfill compaction lead to increased fluid pressure from about 5 years and can peak as high as 25 MPa after about 10 to 20 years when backfill reconsolidation has been completed (Figure 2-2d).

- Analysis of the results shows that high pressure leads to hydraulically induced damage with fluid filtration starting after 6 years at a location 8 m from the drift, whereas the pressure adjacent to the drift is initially relatively low until reconsolidation of the crushed salt backfill (Rutqvist et al., 2014).

In Figure 2-2c we elected to present volumetric moisture content rather than saturation. As shown in Rutqvist et al., (2014), the initial saturation in the backfill is very low (about 2%), leading to an initial volumetric water content of 0.6%. The host rock has much smaller porosity and although fully saturated its volumetric water content is initially 0.2%. Figure 2-2c shows that there are significant non-uniform changes in volumetric moisture content in the backfill, until it gets fully reconsolidated after 6 to 20 years, when the pores are fully saturated but at a very small porosity. These changes in backfill moisture content might be caused by infiltration from the damaged excavation disturbed zone as well as vapor flow movements from the hot inner parts of the backfill with condensations at the cooler outer parts.

Generally, the modeling results indicate that in order to follow the reconsolidation processes, this kind of full-scale field experiment should be prolonged for at least 10 years. After the backfill has reconsolidated, the analysis also shows that significant THM changes can occur in the host rock as a result of thermal pressurization. The type of THM modeling results presented in this study can be used for designing an appropriate monitoring system at a heater experiment. It will help to determine where to install sensors and what type of monitoring techniques to use. For example, Figure 2-2c shows changes in volumetric water content between 0 to 3.5.%, which for a brine lead to significant changes in electric resistivity, which thus could be monitored using electric resistivity tomography.

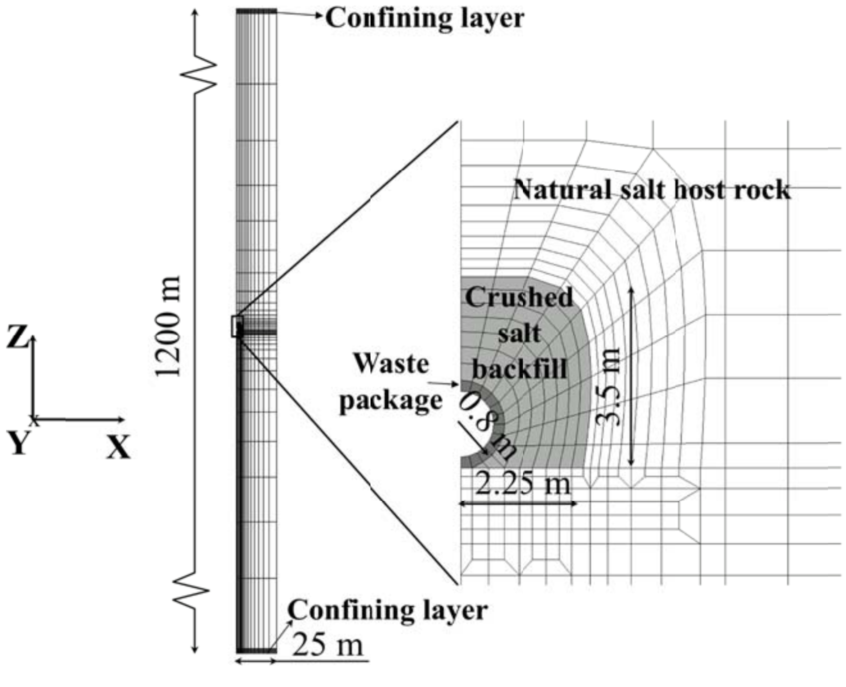
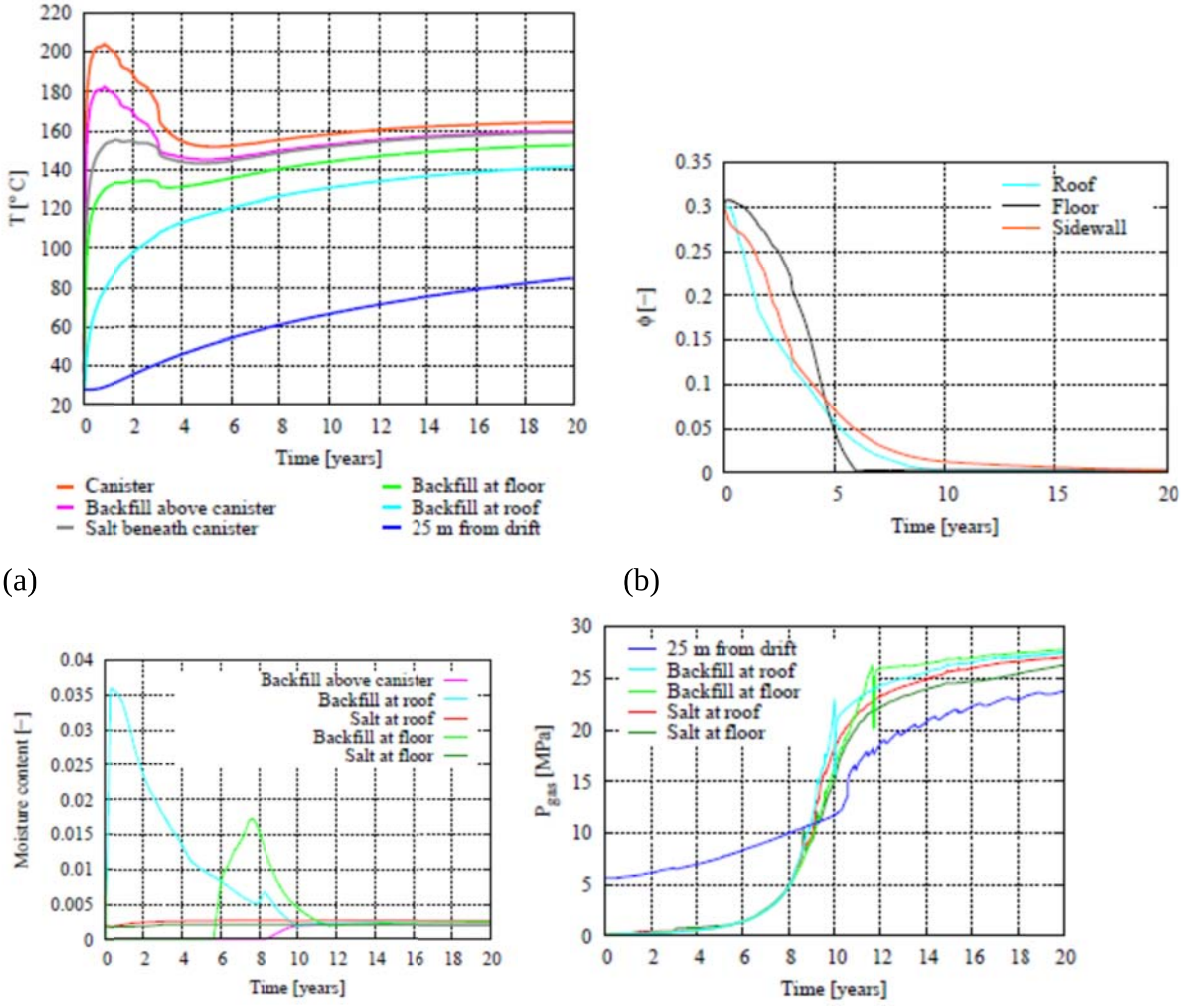


Figure 2-1. Geometry of the generic salt repository studied in Rutqvist et al. (2014), here used for investigating the potential coupled THM responses during a heater experiment.



(a) (b)

(c) (d)

Figure 2-2. Evolution of Geometry of the generic salt repository studied in Rutqvist et al. (2014), here used for investigating the potential coupled THM responses during a heater experiment. (a) Temperature, (b) porosity, (c) moisture content, and (d) pore pressure.

3. RESULTS FROM MODELING TSDE EXPERIMENT AT ASSE MINE, GERMANY

The TSDE (*Thermal Simulation for Drift Emplacement*) test was conducted in the Asse salt mine in Germany in the 1990s to simulate reference repository conditions for spent nuclear fuel in rock salt (Bechthold et al., 1999). This large-scale test is of significant relevance for nuclear waste disposal in salt because extensive research and measurement programs were set up for the experiment. The TSDE test focused on the in-drift emplacement concept. Accordingly, six electrical heaters were placed in two parallel drifts excavated for the purposes of the test in the 800 m level of the mine, in a relatively undisturbed zone. Three heaters were placed in each drift. After installation of the heaters, the test drifts were backfilled with crushed salt (grain size smaller than 45 mm). The test included several observation and access drifts, and more than 200 boreholes for monitoring. The measuring instruments were installed in twenty monitoring cross-sections, both in the heated and non-heated areas. The extensive measurement program included temperature, drift convergence, rock deformation and stress evolution, among others. Heating started in September 1990 and a constant heat load was maintained until the heaters were switched off in February 1999. In addition to providing a vast data base on important phenomena and processes, the TSDE experiment led to (1) an evaluation of the feasibility of the in-drift emplacement concept with multiple barriers, (2) an improved understanding of the backfill and salt rock mass behavior under repository conditions for high-level nuclear waste, and (3) further development of computer codes and constitutive laws required to predict relevant phenomena and processes.

During FY2014, LBNL has commenced coupled THM modeling of the TSDE test using the updated TOUGH-FLAC simulator for large strains and creep processes described in a previous FY2014 milestone report, "*Modeling Coupled THMC Processes and Brine Migration in Salt at High Temperatures,*" FCRD-UFD-2014-000341 (Rutqvist et al., 2014). The open drift phase that preceded the test itself and which lasted 1.4 years has also been modeled in order to determine a suitable initial state for the test phase (8 years). The simulations have been conducted in three dimensions because previous thermal and thermo-mechanical modeling of the TSDE experiment confirmed the need for a 3D model, at least for the determination of the temperature field (Bechthold et al., 1999). Figure 3-1 shows several views and the most important dimensions of our model (half of one drift, with two symmetry planes: one at X=0, across the pillar between the two test drifts, and one at Y=0, across the central cross-section of one test drift).

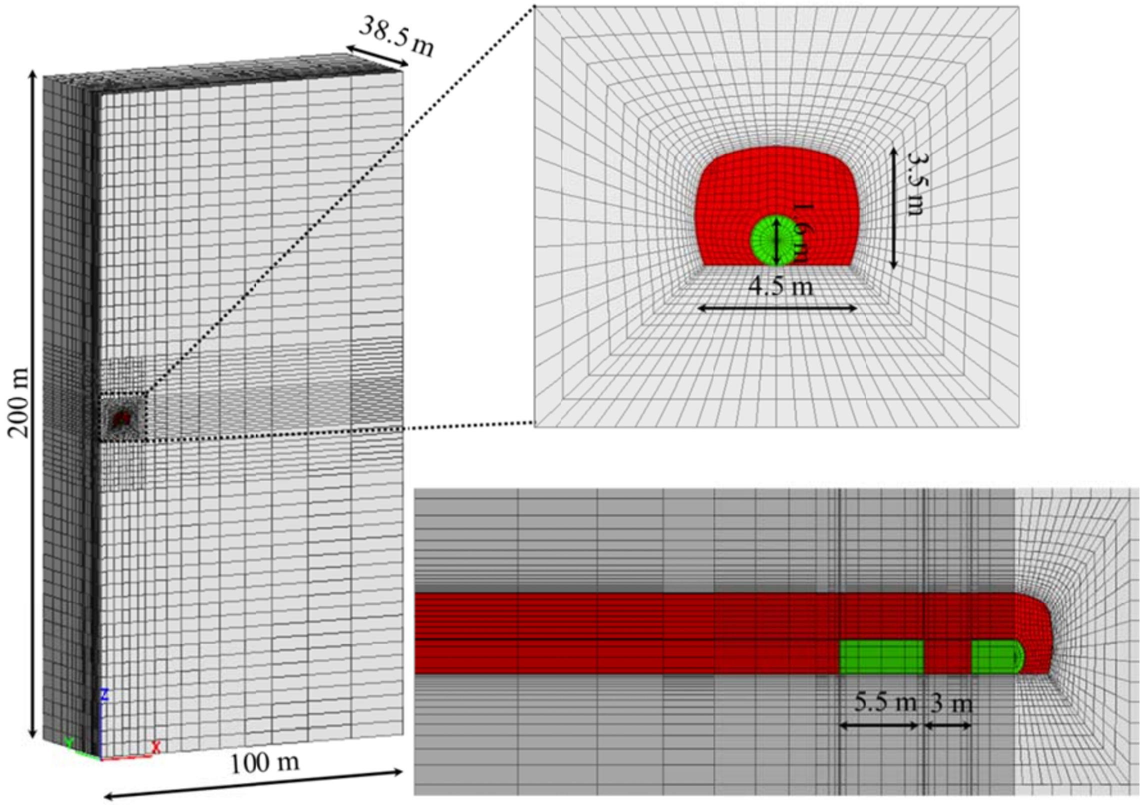


Figure 3-1. Views of the three-dimensional mesh used in the coupled THM simulations and important dimensions.

This modeling effort is being performed in parallel with Prof. Lux's team at Technical University Clausthal, in the framework of an informal benchmark exercise. With respect to previous modeling exercises of the TSDE experiment (Bechthold et al., 1999; 2004; Pudewills and Droste, 2003), we have included transient, damage and healing processes within the natural salt, using the *Lux/Wolters* constitutive model (Wolters et al., 2012), and we have also accounted for hydraulic processes, although the TSDE experiment focused on evaluating thermo-mechanical processes (due to the influence of heating). In addition, we use a customized version of the *cwipp* constitutive model for crushed salt implemented in FLAC^{3D} (Itasca, 2011). In our modified version, density is not a monotonically increasing function, but honors the volumetric strain evolution (Blanco Martín et al., 2014).

Regarding the flow part, a two-phase flow of water and air, by diffusion and convection, is modeled. Heat transport occurs by conduction and convection. TOUGH2 equation-of-state (EOS) 3 is used. Diffusion coefficients are pressure and temperature dependent, and tortuosity is accounted for through the Millington and Quirk model (Pruess et al., 2011). According to *in situ* measurements (Bechthold et al., 1999), the initial stress field in the host rock is 13 MPa, and the initial temperature is 37 ºC. We have assumed initial lithostatic pore pressure conditions. Table 3.1 lists relevant mechanical and flow properties used for the natural and the crushed salt.

Table 3-1. Mechanical and flow properties for the natural salt and the crushed salt.

Property [unit]	Natural salt	Crushed salt
Grain density [kg·m^{-3}]	2,200	2,200
Bulk modulus [MPa]	16,650	150
Shear modulus [MPa]	7,690	70
Lin. therm. expansion coeff. [K^{-1}]	$4\cdot10^{-5}$	$4\cdot10^{-5}$
Initial Biot coefficient [-]	0.003	1
Initial permeability [m^2]	0	$3\cdot10^{-13}$
Initial liquid saturation [-]	50%	2%
Initial porosity [-]	0.2%	35%
Initial specific heat [J·kg^{-1}·K^{-1}]	860	860
Initial therm. cond. [W·m^{-1}·K^{-1}]	5	0.9

The modeling sequence is as follows. First, we model the excavation (instantaneous), and then we perform a coupled THM simulation of the open drift phase (1.4 years). During this phase, the pressure in the drift is set to atmospheric (0.1 MPa). After that, the heater casks and the backfill are emplaced and activated, and we subsequently run a second coupled THM simulation corresponding to the 8-year-long test. In accordance with available data (Bechthold et al., 1999), the initial porosity of the backfill is set to 35 %, and a constant heat load of 6.4 kW is assigned to each heater. This leads to a power output per drift of 19.2 kW. At the beginning of the test phase, we assume atmospheric pore pressure in the backfill and heater cask. Finally, we note that during the modeling of the test phase, one end of the drift is open, to account for ventilation effects.

For brevity, only some relevant results will be presented in this report. We note that the following results correspond to an initial stage of the modeling effort for the TSDE test, in which we have aimed at evaluating the capabilities of TOUGH-FLAC to tackle a large-scale test (global trends well reproduced, computational requirements needed, etc.). For a better agreement between numerical predictions and experimental data, and to understand relevant processes, further simulations will be performed, including a parameter-fitting effort.

The left-hand side plot in Figure 3-2 shows the temperature evolution at four different locations in the heated area (the locations are indicated in the inner sketch). The temperature at the heater surface peaks at 210 ºC five months after the heaters are switched on. Later on, it decreases as the thermal conductivity of the crushed salt increases due to compaction (porosity reduction). Backfill compaction is mainly triggered by drift closure, which is in turn enhanced by the temperature increase. After about 5 years, temperatures in the heater cask area reach a steady state, while they continue to increase at further distances from the heater. As can be seen, the temperature evolution at the heater cask is slightly overestimated during the first five years of heating, although the predicted temperature does decrease as the backfill compaction moves forward. The measured and predicted evolution of temperature in the rock salt beneath the drift (heated area) is displayed in the right-hand side plot in Figure 3-2. It can be seen that the temperature decreases with depth. As the plot shows, the temperatures are overestimated in the heater cask and within the first 1.2 m below the drift floor. The temperature stabilizes after about 5 years of heating.

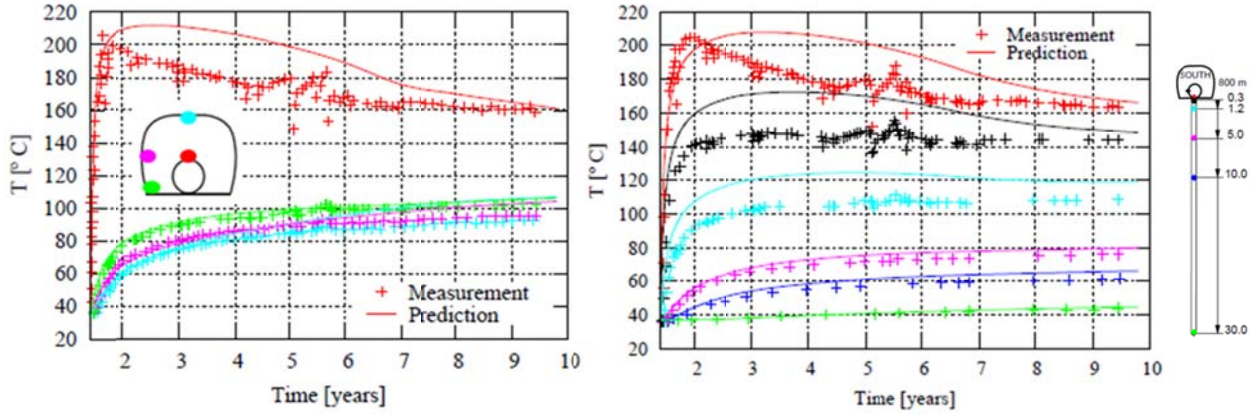


Figure 3-2. Left: temperature evolution at the heater cask surface and at the backfill around a central heater; Right: rock temperatures beneath the drift in the heated area

On the other hand, in the non-heated area (left-hand side plot in Figure 3-3), the temperatures do not reach a steady state. In this case, heat is not only transferred by conduction through the rock salt, but also through the backfill in lateral direction following the drift. As this figure shows, the match between experimental and predicted values is more satisfactory in the non-heated area than in the heated area.

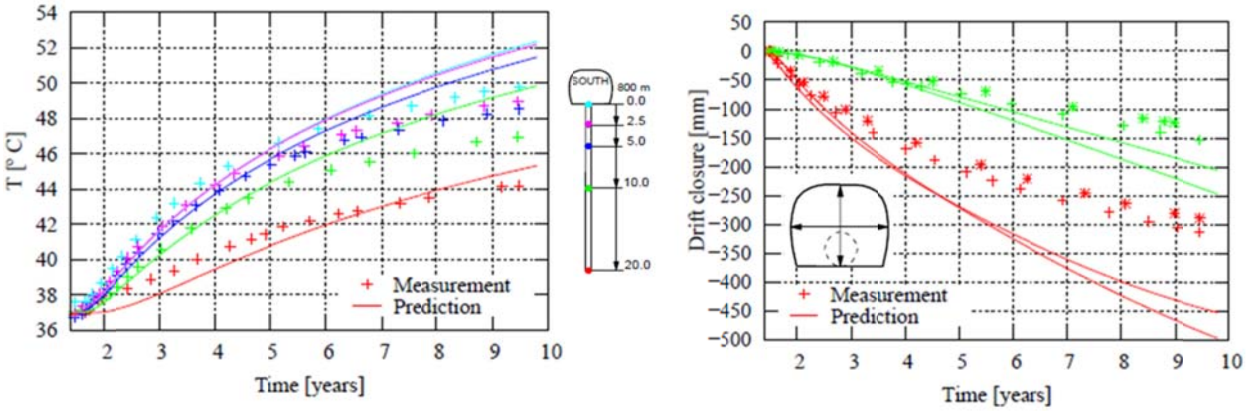


Figure 3-3. Left: rock temperatures beneath the drift in the non-heated area; Right: drift closure in the heated area (red values) and non-heated area (green values)

The right-hand side of Figure 3-3 displays the drift closure over time, both in the heated area and in the non-heated area. Drift closure is calculated from horizontal and vertical convergence data. In the heated area, the drift closure rate is very high at the beginning, but decreases over time as the backfill gets progressively compacted. As compaction moves forward, the backfill densifies, stiffens and provides increased mechanical support at the drift walls. On the other hand, in the non-heated area the closure rates do not change significantly during the test. As the figure shows, the numerical predictions overestimate the experimental data. One possible reason for this overestimation could be that the experimental creep strain rate of the natural salt is slower than the modeled creep strain rate. Another reason could be that the observed response of the crushed salt during the TSDE experiment is stiffer than predicted by the *cwipp* model. We are currently performing additional simulations to determine the most likely reason for this overestimation.

Overall, while the most important features are captured by the code and constitutive relationships used, more insight needs to be gained to understand the differences observed between measurements and numerical results. These differences could be caused by some simplification in the constitutive relationship used to model crushed salt compaction, or by a modeled creep strain rate for natural salt faster than measured. Further three-dimensional simulations will be performed. On the other hand, features that are currently accurately captured include the evolution of crushed salt thermal conductivity during compaction and the evolution of temperature towards a steady state in the heater surface and nearby backfill and rock mass.

4. DUAL-CONTINUUM APPROACH FOR BRINE MIGRATION MODELING UNDER THERMAL AND HYDRAULIC GRADIENTS

For the analysis in support of brine migration field experiments under high temperature, LBNL is developing a dual-continuum modeling approach that accounts for brine migration through both interconnected intergranular (i.e., intercrystalline) pore spaces and isolated fluid inclusions (i.e., intracrystalline brine inclusions), considering both pressure and temperature gradients. Given the strong thermal gradients that are expected to exist in salt formations hosting high-level radioactive waste repositories, the applicability of a single-continuum approach, based on the assumption of equilibrium between the pore fluid and surrounding solids, is questionable. A dual-continuum approach, in which the pore fluid and solids are treated as two separate but interacting continua occupying the same physical space, one can resolve the strong gradients at the fluid-solid interface more efficiently.

Figure 4-1 shows a schematic diagram of the proposed dual-continuum model, including the interconnected pore space and the intracystalline inclusions, and the various fluxes and inter-continuum exchanges (Rutqvist et al. 2014). In this dual-continuum model, one continuum represents the connected intercrystalline pore space (where flow and transport is mostly controlled by pressure gradients, and molecular and thermal diffusion) and the other represents the intracrystalline inclusions (where the primary transport mechanism is temperature-driven solubility changes). Because both media are treated as separate systems, flow and transport processes are described by two sets of conservation equations (one set each for each of the two continua), which are coupled through suitably defined exchange terms. To address inclusion migration behavior at the grain boundaries, we intend to adopt a probabilistic approach. In this approach, an inclusion after reaching the grain boundaries would drain into the inter-connected pore space continuum with a probability *p*, or bypass it and migrate into the neighboring grains with a probability of 1-*p*. The plan is to implement such an advanced brine-migration dual-continuum model into the TOUGH2 and TOUGH-FLAC simulators, and then validate the brine-migration model and its implementation against experimental laboratory data. The dual-continuum model and TOUGH2 can then be used to investigate and design field heater experiments to model potential brine release and migration under the high thermal gradient and high temperature evolutions.

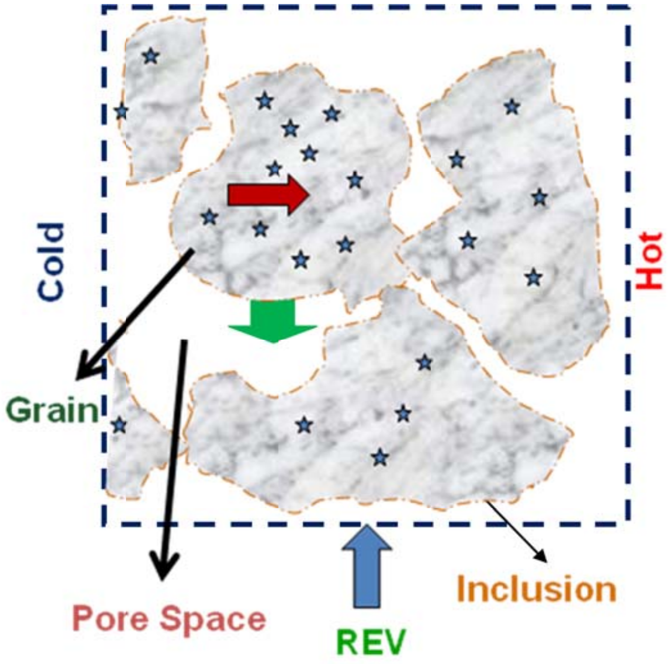


Figure 4-1. Schematic diagram showing the interconnected pore space and the intracystalline inclusions within a representative elementary volume (REV) in a dual-continuum conceptualization of salt formations. Figure also shows the various fluxes and inter-continuum exchanges.

5. SUPPORT OF FIELD TEST PLANNING AND DOCUMENTATION

In FY2014, UFD initiated planning activities for field testing of processes relevant to the safety of disposing heat-generating waste in deep salt formations. The purpose of these planning activities is to ensure that such field testing has clearly defined objectives, that a consensus is reached on those objectives, and that the activities are integrated and collaborative. LBNL participated in these planning activities as follows:

1) LBNL co-authored Milestone "*Framework for Underground Research in Salt*," M4FT-14LA0818066 [Draft], due 9/26/2014. The purpose objective of this framework document is to facilitate objective, rigorous, and transparent science and engineering testing in a salt URL for the purpose of studying the feasibility of disposal of heat-generating waste in salt formations.

2) LBNL provided input and also review comments to Milestone "*Test Plan for Mechanical and Hydrological Characterization of the Near-field Surrounding Excavations in a Geologic Salt Deposit*," M4FT-14LA08180610, due 9/26/2014. Excavations created in salt present a unique opportunity to measure and characterize in situ development of the excavation disturbed zone (EDZ). The purpose of the test plan is to describe how to characterize and quantify the time-dependent mechanical behavior and hydrologic response of salt host rock affected by excavation.

6. CONCLUDING REMARKS

In FY2014, LBNL's work related to modeling and field test planning activities included technical review of framework documents and test plans, participation in workshops associated field test planning, and model development and application for investigating coupled THMC processes at the field-experiment spatial and temporal scales and potential monitoring techniques.

In this report, we first examined previous generic repository modeling results, focusing on the first 20 years to investigate the expected evolution of the different processes that could be monitored in a full-scale heater experiment. The simulation shows that significant multiphase fluid flow processes occur both within the backfill before reconsolidation as well as in the host rock, in addition to the thermal-mechanical processes affecting the reconsolidation of the backfill as well as damage evolution and healing of the host rock. Generally, at least 10 years of heating and monitoring would be required to monitor the reconsolidation of this kind of full-scale experiment to completion. After 10 years, thermal pressurization in the host rock may cause fluid movements by opening of grain boundaries for fluid flow.

We also present results from ongoing modeling of the TSDE experiment, a heater experiment on the in-drift emplacement concept at the Asse Mine, Germany. The results presented are an initial stage of the modeling effort for the TSDE test, in which we have aimed at evaluating the capabilities of TOUGH-FLAC to tackle a large-scale test (global trends well reproduced, computational requirements needed, etc.). Further simulations will be performed (including a parameter-fitting effort) to achieve better agreement between numerical predictions and experimental data, and to better understand relevant processes. Nevertheless, the results show that we are able to model the coupled THM responses capturing trends of the measured temperature and mechanical deformations. The overall thermal and mechanical responses at the TSDE are similar to the modeling of the generic repository case, with peak temperature reached in a few years and consolidation taking more than 10 years.

We are currently developing a dual-continuum approach that accounts for brine migration through both interconnected intergranular (i.e., intercrystalline) pore spaces and isolated fluid inclusions (i.e., intracrystalline brine inclusions), considering both pressure and temperature gradients. The plan is to implement such an advanced brine-migration dual-continuum model into the TOUGH2 and TOUGH-FLAC simulators, and then validate the brine-migration model and its implementation against laboratory experimental data.

In FY2015, LBNL plans to continue modeling and field test planning activities including technical review of test plans, participation in workshops associated field test planning, and model development and application for investigating coupled THMC processes at the field-experiment spatial and temporal scales and potential monitoring techniques.

- Continue our modeling efforts on the Asse Mine TSDE experiment, in collaboration with Claustal Technical University, Germany.
- Extend modeling from THM to THMC processes considering salt precipitation and dissolution.
- Implement proposed dual-continuum model into TOUGH2 and test it for modeling thermally driven brine migration and investigate the roles of intercrystalline flow versus intracrystalline brine inclusions on the overall brine migration.

- Conduct coupled geomechanical model simulations to support the design of any proposed heater experiment in salt.
- Continue to provide input into characterizing and monitoring methods and test plans for in situ testing (mine-by testing, heater testing) of relevant THM processes in salt.

ACKNOWLEDGMENTS

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