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Analyzing Field Data from the Brine Availability Test in Salt (BATS): A High-Resolution 3D Numerical Study

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The disposal of heat generating nuclear waste is a worldwide concern. Salt formations have been investigated as candidate disposal host rocks for heat-generating nuclear waste for decades. However, brine availability is influenced by heat and can affect the evolution of a nuclear waste disposal facility in salt. For example, brine migration is a potential radionuclide transport vector and brine leads to corrosion of waste forms and waste packages. To better understand brine migration in heated salt, he US Department of Energy's generic disposal research campaign is conducting borehole heater experiments are being conducted underground at the Waste Isolation Pilot Plant (WIPP) near Carlsbad, New Mexico. A crucial component of this field test is utilizing numerical models to better understand the system and the data being collected. Meshing and modeling heated, multiphase flow in porous media is a complex and computationally demanding problem. Here we use Voronoi meshing to accurately reproduce the complex 3D geometry of the Brine Availability Test in Salt (BATS) heater test at WIPP. Voronoi elements guarantee accurate fluxes in finite volume simulations, and their distribution is optimized to allow efficient simulation of heat and brine migration during the heating/cooling cycles of the BATS 1a heater test.

1 Introduction

1.1 Background

The United States has investigated disposing of radioactive waste in geologic salt since the 1950s when Hess et al. (1957) recommended direct disposal of liquid reprocessing waste into salt caverns. Since, underground field studies have investigated phenomena that could occur in a mined repository in salt at several sites across the United States, including: Project Salt Vault (Bradshaw and McClain, 1971), Avery Island (Llewellyn, 1978; Just, 1978; Van Sambeek, 1981), Deaf Smith (Pfeifle et al., 1983a; 1983b), and the Waste Isolation Pilot Plant (WIPP) (e.g., Munson et al., 1979a; Krause, 1981; Stormont, 1984; Molecke and Sorensen, 1988; Krumhansl et al., 1991, Franckel et al., 1999; Hardy and Holcomb, 2000), which is a deep geologic repository for non-heat generating transuranic defense waste near Carlsbad, NM.

Salt is a potentially effective disposal medium for heat-generating radioactive waste such as spent nuclear fuel due to its low permeability (Beauheim and Roberts, 2002) to brine transport and high thermal conductivity relative to other candidate disposal media, such as clay or granite. While undisturbed rock salt has almost unmeasurably low porosity and permeability, upon drift or borehole excavation a damaged region develops surrounding the excavation (Borns and Stormont, 1989). This disturbed rock zone (DRZ) around boreholes or access drifts introduces significant changes impacting the near-field transport of brine and gas through the

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salt (Stormont, 1997). The mechanical damage is caused by stress concentration near the excavation, which leads to increased permeability and porosity of the salt through a network of induced fractures which provide high-permeability pathways for brine transport (Kuhlman et al., 2017). Since brine migration is a potential radionuclide transport vector, understanding and characterizing near-field conditions (i.e., DRZ) and processes is an important initial condition to assessing the long-term safety of the system. The development of the DRZ also leads to significant changes to the stress and pore pressure within the salt. Intergranular brine will migrate towards the low-pressure drift or borehole via the new halo of connected porosity and permeability comprising the DRZ (Figure 1). The addition of heat from a waste package can liberate additional intra-crystalline brine: (1) high temperatures can cause decrepitation (i.e., rupture) of fluid inclusions (Roedder and Belkin, 1979) and (2) an elevated temperature gradient drives fluid inclusions to migrate towards the heat source (Roedder and Belkin, 1980). Once liberated from within crystals, this fluid becomes more mobile as inter-crystalline brine, which flows through new interconnected fracture network of the DRZ down a pressure gradient. These excavation- and heat-induced changes within the salt cause a near-excavation higher permeability pathway to allow inter- and intra-crystalline brine (enhanced from the introduction of heat) to migrate towards the excavation, leading to a complex short-term and near-field flow system.

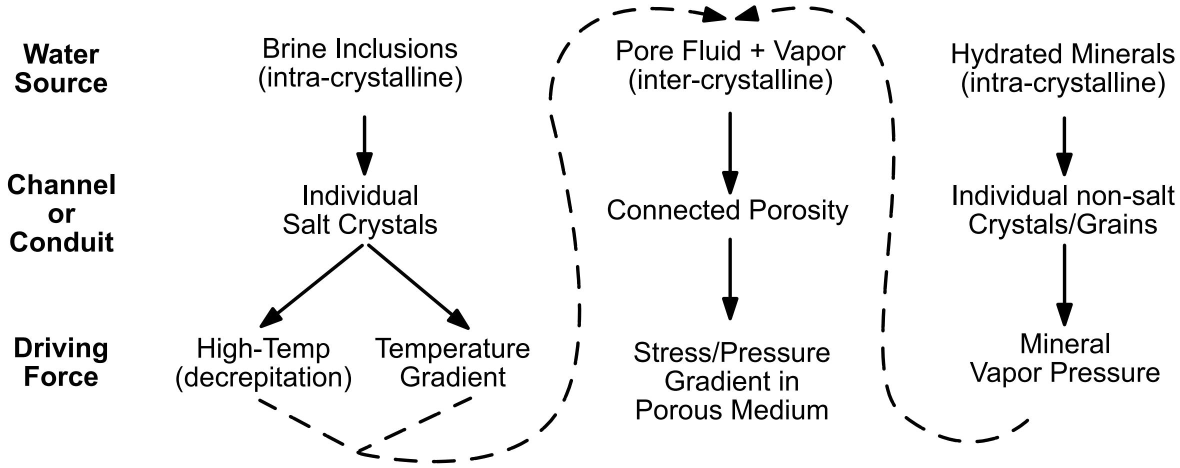

Figure 1. Relations between brine types and flow mechanisms in salt (adapted from Shefelbine (1982)).

1.2 Brine Availability Test in Salt (BATS)

To better quantify the effects of the DRZ and understand how higher temperatures impact brine availability and migration within salt, several heated brine migration tests have been implemented since the 1960s to investigate these engineered systems, including tests as part of Project Salt Vault (Bradshaw and McClain, 1971), Avery Island (Llewellyn, 1978; Just, 1981; Van Sambeek et al., 1983), WIPP (Munson et al., 1997), and Asse II (BMWI, 2008). These studies were each different, but they all highlighted the difficulty in studying brine availability and migration within salt and the heterogeneity associated with the DRZ around drifts. Understanding and quantifying heat and mass transport in salt during a salt heater test requires advanced understanding and subsequent complex numerical models of the thermal-hydrological-mechanical system.

The Brine Availability Test in Salt (BATS), hosted at the WIPP courtesy of the US Department of Energy (DOE) Office of Environmental Management, is part of the DOE Office of Nuclear Energy's generic (i.e., non site-specific) disposal research program. BATS is a meter-scale borehole heater test, with the goals of: (1) improving the understanding of brine availability and brine chemistry in the DRZ for bedded salt; (2) collecting data for validating numerical models, populating constitutive models, and improving process model understanding; and (3) revitalizing in-house expertise at participating institutions in implementing *in situ* experiments in salt (Kuhlman et al., 2017).

The experimental setup for BATS includes two arrays of boreholes, each with a 4-m long, 12-cm diameter horizontal, central heater borehole surrounded by an array of thirteen sub-parallel sampling and monitoring boreholes. One array was heated, the other was monitored at ambient temperature. In January 2020, the first phase of the BATS heating experiment began. The heater was set to a constant temperature of ~95°C for 28 days, the heater was then shut off and the salt was monitored while cooling for 13 days (Kuhlman et al., 2020). During the 41-day experiment temperature data and brine inflow rate were measured at a high frequency (15-minute averages), along with daily electrical resistivity tomography surveys, continuous monitoring of acoustic emissions, and high-frequency water isotopic and gas composition data by in-drift spectroscopy.

To further understand the field data collected during the BATS field test, we utilize a high-resolution, three-dimensional (3D) thermal-hydrological (TH) model to analyze the temperature distribution within the DRZ and intact salt at WIPP. The finite-volume code PFLOTRAN (Hammond et al., 2014) was used to simulate mass and heat transport within the two-phase (air & water) system. An additional challenge added to this modeling study is the geometric complexity of the BATS field experiment, which is difficult to represent with block hexahedral elements. While hexahedral meshes can be deformed to capture some of the configurational complexity of the field test, the boreholes and drift require some grid cells be badly scaled leading to non-orthogonality (i.e., element faces not perpendicular to the line connecting adjacent element centers) that can cause flux errors in finite volume meshes leading to mass no longer being conserved when fluid flows between elements. To avoid this potential numerical issue, here we use VoroCrust (Abdelkader et al., 2018; 2020), a fully automated Voronoi meshing software that has been adapted to create simulation grids for PFLOTRAN in complex geological systems.

2 Methodology

This study combines Voronoi meshing of the BATS field test and TH numerical modeling to investigate the influence of the fractured nature of the DRZ on brine flow and temperature migration within bedded salt. The current model represents the BATS field experiment, where a 69-cm long interval 2.75 meters deep into in the central borehole (Figure 2) is heated to a constant temperature while temperature is monitored at 66 thermocouples (72 total thermocouples in the heated array, 66 of which produced useable data) grouted into satellite boreholes around the heater (see Kuhlman et al. (2020) for sensor locations and detailed test and data descriptions). Not all 14 boreholes were explicitly meshed, but the permeability and porosity disturbance associated with each excavation were accounted for by superimposing decaying power-law relationship away from the drift (Figure 3). The thermal and hydrological properties of the salt (Table 1) are taken from Jayne and Kuhlman (2020), where a suite of 1D analytical solutions and TH models were utilized in conjunction with Markov chain Monte Carlo methods to constrain the reservoir parameters at the BATS field experiment by matching both temperature and brine flow field data.

Table 1. Model properties for the 3D BATS heater test simulation. Permeability and porosity vary by distance away from the drift and each borehole (see Figure 3).

Reservoir Parameters		**Mualem – Van Genuchten Relative Permeability**		**Van Genuchten Capillary pressure**	
Initial Temperature (°C)	29.5	**λ**	0.6	**λ**	0.6
Permeability (m^2)	Varies	S_{lr}	0.2	S_{lr}	0.2
Porosity (-)	Varies	S_{ls}	1	**α** (Pa^{-1})	10^{-6}
Thermal Conductivity W/m°C	Varies	S_{gr}	0.2	S_{ls}	0.999
Heat Capacity J/kg°C	620				

2.1 Voronoi Meshing

The workflow used here to create a Voronoi mesh for PFLOTRAN used two programs; LaGriT (LANL, 2017) and Vorocrust (Abdelkader et al., 2018; 2020). LaGrit is a library of mesh generation and optimization tools in two and three dimensions that was used to create borehole- and drift-bounding surfaces for input into Vorocrust. Figure 2A illustrates the surfaces created in LaGriT, which consists of the BATS drift and a single heater borehole (the heater and packer extents are also defined in LaGriT). The model domain only includes a 5 m high by 0.5 m wide section of the drift because the area of interest is the salt surrounding the borehole, but the drift is included as a boundary condition. Vorocrust creates a 3D Voronoi mesh (Figure 2B). Figure 2C and 2D show slices down the center of the model domain parallel to the heater borehole, while Figure 2D is a zoomed-in section of the heater borehole to illustrate the fine mesh within and around the borehole (the smallest element has a volume of 6.0×10^{-6} m^3). Vorocrust can resolve the mesh around possibly curved areas of interest while coarsening rapidly away from the area of interest, to reduce the total number of elements and computational burden. Voronoi elements, by construction, are the optimal elements for finite volume simulators, like PFLOTRAN. The current model domain presented is 40 m × 40 m × 40 m consisting of 135,810 elements. Unlike hexahedral meshes, Voronoi meshes do not have a fixed number of connections per element, which leads to a higher connectivity than structured meshes, resulting in more poorly conditioned residual matrices. To address this issue, we used a constrained pressure residual pre-conditioner, which aids with the added numerical challenges associated with a Voronoi mesh (Park et al., 2021).

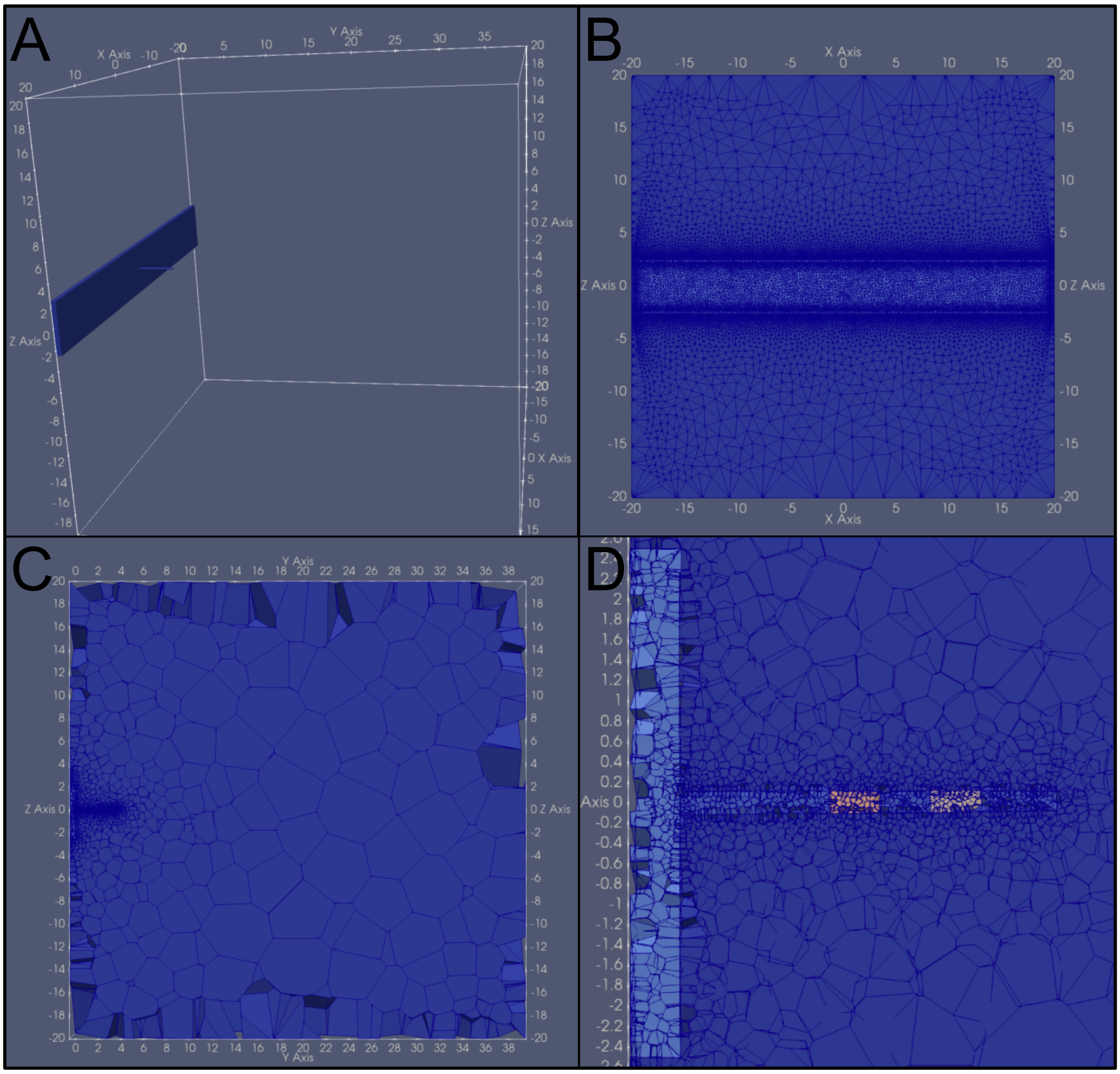

Figure 2. Illustrates the: (A) surface mesh created with LaGrit, featuring a drift and a single heater borehole, (B) an XZ view of the meshed model domain, highlighting mesh refinement around the drift shown in light blue (element boundaries are dark blue lines), (C) a YZ slice through the center of the model domain to highlight areas of high refinement (near the drift and borehole) and the coarsening of the mesh away from areas of interest, and (D) a zoomed in view of the drift, heater borehole, packer location (orange), and heater location (tan).

2.2 DRZ Permeability and Porosity

While thermal, hydrological, and mechanical properties of bedded salt have been studied extensively at the WIPP site and previous salt underground research laboratories, the steep spatial gradient of state variables and material properties across the DRZ (e.g., the pores are air-filled at atmospheric pressure in the drift and brine-filled to lithostatic pressure in far field, as little as 5 excavation radii away – Beauheim and Roberts, 2002) makes accurate characterization and simulation of these regions difficult. In numerical studies it is difficult to constrain and/or define the DRZ and intact salt within the model domain and it is commonly handled by considering the DRZ and intact salt to be two separate domains with a sharp boundary between the two. Here we assume that the transition from DRZ to intact salt is gradual and is defined by a decaying power law relationship. Figure 3A illustrates how permeability decays away from the drift by $k = k_0 \left[\frac{r}{r_0}\right]^{-7.5}$, where k is permeability [m²] and k_0 is maximum permeability at the excavation boundary (10^{-14} m²), r is distance from the excavation [m], and r_0 is the excavation radius (drift radius is 2.5 m, borehole radii were 6 and 2.5 cm). The permeability of any element in the model domain was then a superposition of power-law distribution contributions from the drift and all 14 boreholes, based on the distance from each excavation to the element. Similarly, porosity decays away from the drift and borehole (Figure 3B), which is defined by $\phi = \phi_0 \left[\frac{r}{r_0}\right]^{-3.5}$, where ϕ is porosity, and ϕ_0 is the highest porosity near the drift (10%).

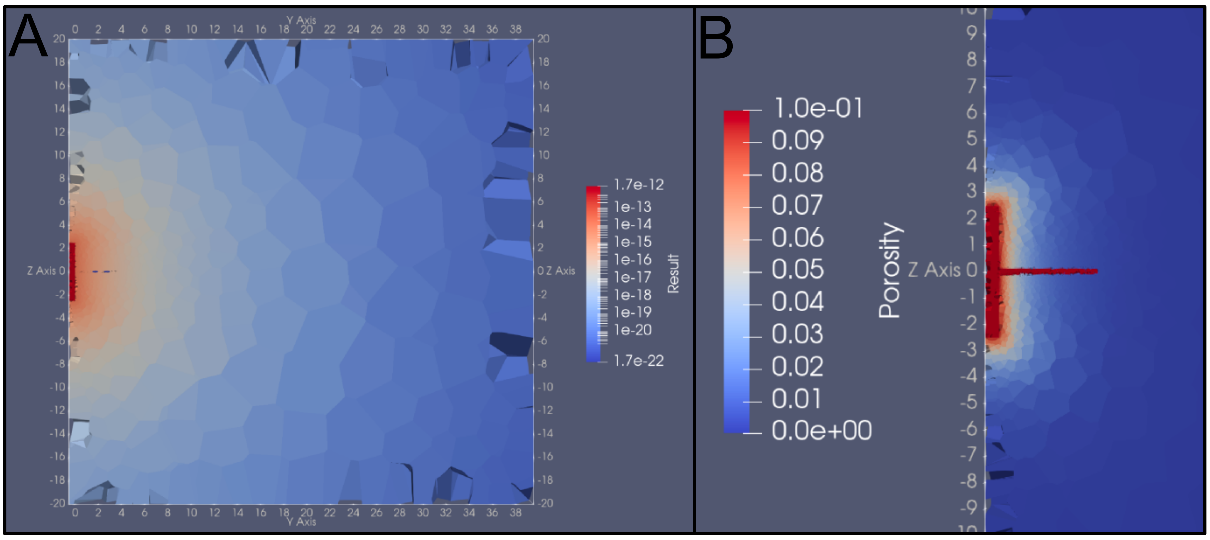

Figure 3. Average permeability and porosity distribution within the DRZ and intact salt. A and B) YZ slice through the center of the domain to show how average permeability (A) and porosity (B) decay away from the drift.

2.3 Thermal Conductivity

Intact salt has higher a thermal conductivity (>6 W m^{-1} K^{-1} at 20°C) than most other rocks and it is strongly temperature-dependent (Raymond et al., 2021; Kuhlman et al., 2020). As temperature increases the thermal conductivity decreases and this can play an important role in accurately modeling a salt heater test. To account for this temperature dependence, we have use a cubic polynomial temperature dependent thermal conductivity model show in Figure 4.

$$k_T(T,S_l) = k_{T,\text{dry}} + \sqrt{S_l}(k_{T,\text{wet}} - k_{T,\text{dry}})\left[1 + \beta_0 T + \beta_1 T^2 + \beta_3 T^3\right]$$

where the thermal conductivities at liquid saturation (S_l) of 1 and 0 are $k_{T,\text{wet}} = 7$ W m^{-1} K^{-1} and $k_{T,\text{dry}} = 4.5$ W m^{-1} K^{-1}. The three cubic polynomial coefficients used were -4.53398E-3, 1.41580E-5, and -1.94840E-8, based on fits against thermal conductivity data from BATS cores (Kuhlman et al., 2020).

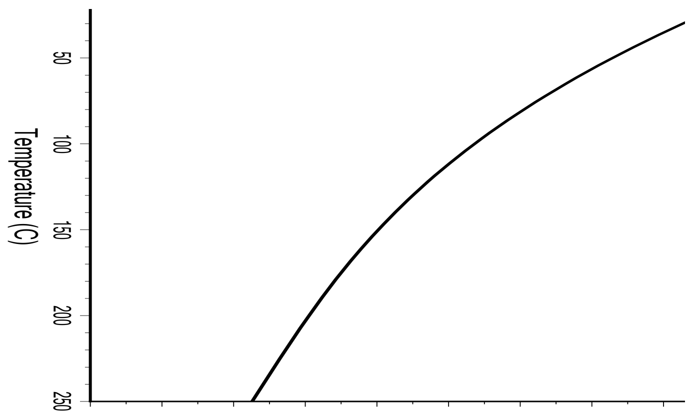

Figure 4. Temperature dependent thermal conductivity model (at full liquid saturation) for intact salt.

2.4 Initial Conditions

The computed initial pressure and saturation profiles for the model domain are shown in Figure 5. To create the initial distribution a preliminary simulation was run with the drifts and borehole set at atmospheric pressure and 99% gas saturation, and model domain was initialized at fully liquid saturated at 12 MPa. The borehole and drift conditions are held constant and the edges of the model domain at $z = 20$ m, $z = -20$ m, and $y = 39.5$ m are no-flow and insulated boundary conditions. To evolve representative initial pressure and saturation conditions for BATS, the preliminary simulation ran to 180 days, which is roughly the amount of time between the BATS boreholes being drilled and the beginning of the heater test, shown in Figure 5.

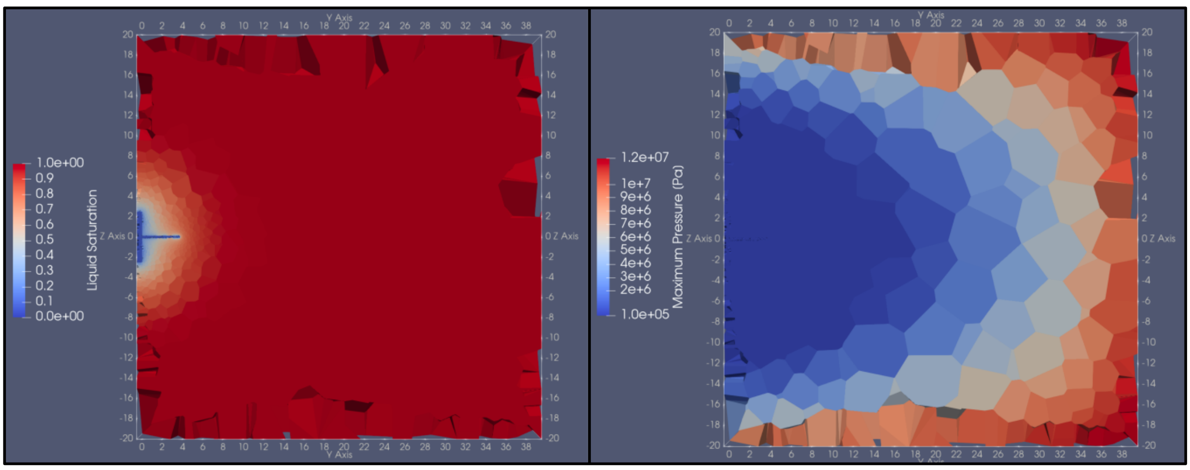

Figure 5. Initial conditions (end of preliminary simulation) for liquid saturation (left) and maximum pressure (right). The YZ slices are parallel to the heater borehole and perpendicular to the drift.

The results of this preliminary simulation are then used as initial conditions for the BATS heater test experiment. The simulator used for this study is PFLOTRAN (Hammond et al. 2014), an open source, state-of-the-art massively parallel subsurface flow and reactive transport code. The simulation covers 41 days, 28 days where a heater is run at constant temperature (~95°C) and 13 days after the heater is shutoff.

3 Results & Conclusions

The preliminary modeling of the BATS heater test using a 3D Voronoi mesh are illustrated by matching the temperature at six different thermocouples in Figure 6. The six thermocouples chosen were selected based on the proximity of an element center to the location of the thermocouples in the field. Figure 6 illustrates that four of the six thermocouples reproduce the temperatures measured in the field accurately, while the temperature at HE1-TC3 and HF1-TC2 is slightly overpredicted by the current model. While these results are preliminary, they do provide confidence in the current workflow and model conceptualization presented here. Further work on matching brine inflow and the variability of the exponents specifying the permeability and porosity distribution within the DRZ will further the robustness of the current workflow and the heuristic nature of numerical models.

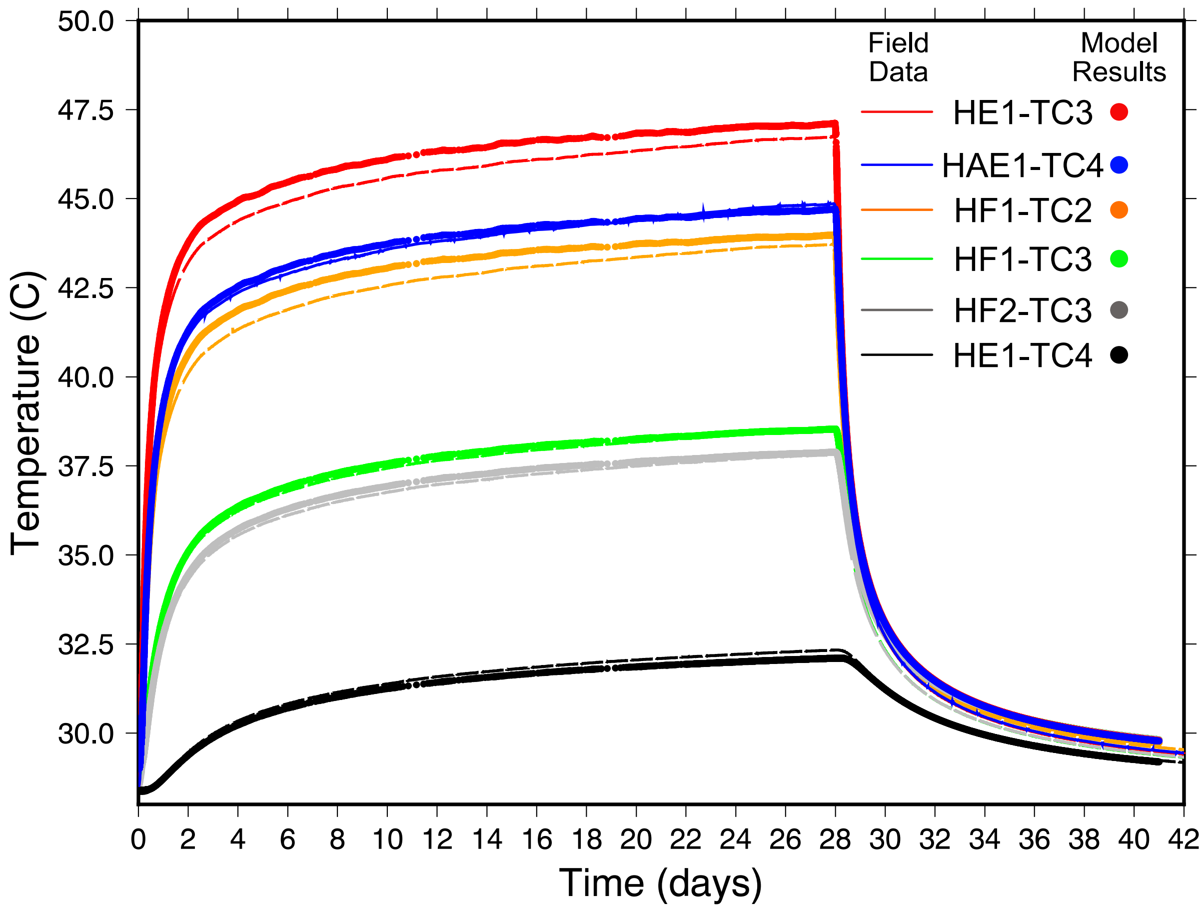

Figure 6. Numerical modeling results for measured temperature at six thermocouples during the BATS heater test.

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