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To:
United States Nuclear Waste Technical Review Board
2300 Clarendon Boulevard, Suite 1300, Arlington, VA.

At the request of the U.S. Nuclear Waste Technical Review Board (NWTRB), I attended and provided technical feedback on presentations by the U.S. Department of Energy (DOE) researchers at the "Workshop on Recent Advances in Repository Science and Operations from International Underground Research Laboratory Collaborations" held in San Francisco, CA on April 24-25, 2019 and the "Fact Finding" meeting held in Las Vegas, NV on February 26, 2019 that supported the workshop. My technical feedback is focused on DOE's simulations of coupled thermo-hydro-mechanical processes in bentonite used in the engineered barrier system component of an underground geologic disposal facility, which were compared with data collected from different field-scale experiments at international facilities (e.g., FEBEX, Bure, etc.) along with laboratory-scale experiments (gas breakthrough). They are also related to simulations of future projects such as HotBENT that will involve heating of bentonite materials to higher temperatures than those encountered in previous field-scale experiments. My technical feedback to the NWTRB from my review of these presentations is summarized in the following points:

1. Parameter calibration is a major challenge for coupled thermo-hydro-mechanical (THM) models for unsaturated bentonite in engineered barrier systems, especially as many of model parameters are sensitive to the initial conditions and structure of emplaced bentonite and are also coupled with changes in void ratio and temperature. Although it is reasonable and cost-effective to collect data from available sources in the literature, confidence in analyses may be gained through coordinated calibration experiments or inverse analyses of physical modeling experiments. Initial conditions (dry density and gravimetric water content) of the bentonite should be carefully quantified to provide a reference for simulations, and constitutive properties should be developed for these initial conditions.
2. Thermo-elasto-plasticity is an important topic that should be considered in THM modeling of unsaturated bentonite, especially when encountering higher temperatures as part of the HotBENT project. Previous experimental studies on unsaturated, compacted bentonites have found that there may be plastic thermal expansion of initially unsaturated bentonite during drained heating (e.g., Romero et al. 2005). Further, other experimental studies found that the thermal expansion of bentonite may transition to plastic thermal contraction at higher temperatures for some initial conditions (e.g., Tang and Cui 2009). Plastic thermal

volume changes could lead to permanent changes in thermal and hydraulic properties and also may affect the bentonite hydration and corresponding swell pressure. Consideration of thermo-elasto-plasticity in THM modeling may result in improved model fidelity. Most thermo-elasto-plastic models available in the literature are based on the model of Hueckel and Borsetto (1990), which has since been extended to unsaturated conditions in studies like Francois and Laloui (2008). Francois and Laloui (2009) applied a thermo-elasto-plastic model to the ATLAS in-situ test. Dupray et al. (2013) applied a thermo-elasto-plastic model to the 1st phase of the FEBEX experiment and obtained good compliance, and their model was used further by Qiao et al. (2017) to simulate the second phase. These models are based on thermo-elasto-plasticity concepts of Hueckel and Borsetto (1990), but alternative thermo-elasto-plastic models are available in the literature that may be considered for compacted bentonite. For example, Coccia and McCartney (2016a, 2016b) discuss different constitutive modeling approaches for thermal volume change of unsaturated soils including thermally-induced secondary compression (creep). However, these constitutive modeling approach need to be verified and potentially improved for the higher temperature ranges expected in HotBENT.

3. Several couplings between different variables may be encountered during thermo-hydro-mechanical processes in unsaturated bentonite, and these issues may become more important under higher temperatures like those expected in HotBENT. It may be relevant for DOE to consider these couplings in future modeling efforts if they are not already. Examples of these coupling include:
    a. Volume change due to either swelling/shrinkage during wetting/drying or expansion/contraction due to heating can lead to coupled changes in the thermal and hydraulic properties of bentonite. For example, denser soils have higher thermal conductivity than looser soils (e.g., Brandon and Mitchell 1989; McCartney et al. 2013). This effect is superimposed atop the effect of the degree of saturation on the volume change and may play an important role in the heat transfer processes.
    b. An important issue not considered in current THM analyses of the engineered barrier system is the effect of temperature on the soil-water retention curve (SWRC) or the hydraulic conductivity. The air-water surface tension, water-solid contact angle, and water viscosity are all dependent on temperature. Villar and Gomez-Espina (2007) found that a significant reduction in water retention may occur during heating from 40 to 102 °C. As the shape of the hydraulic conductivity function may be related to the SWRC, this is a critical need. SWRC models for elevated temperature are available in the literature (e.g., Grant and Salehzadeh 1996), but these have not been applied to bentonites.
    c. The use of the van Genuchten model to represent the SWRC of bentonites may lead to issues at high suction values. A new SWRC model that considers adsorption and capillarity mechanisms of water retention was developed by Lu (2016) that may lead to improved behavior at high suctions. Following on this comment, estimating the shape of the hydraulic conductivity function (HCF) from the SWRC should also be carefully evaluated.
    d. Coupling between the SWRC and the thermal properties is another important issue to consider in coupled THM models. These include thermal conductivity function models like Lu and Dong (2015), which can also be extended to the volumetric heat capacity function (Baser et al. 2018).

   e. Although it is well known that temperature is a driver for vapor diffusion in soils due to the dependence of the saturated vapor concentration in the gas phase on temperature, temperature can also lead to effects on the magnitude of the vapor diffusion coefficient in air. Consideration of this variable may better match the thermally-induced drying observed in the FEBEX experiments. Examples of studies considering temperature effects on the vapor diffusion coefficient are Smits et al. (2011) and Baser et al. (2018), although these focused on thermally induced water flow in sands and silts and may be different than compacted bentonite.

4. The rate of hydration of the bentonite should be carefully considered on a site-specific basis for the permeability and hydrostatic pressure in the host rock. The rate of hydration in the FEBEX experiment seems to be slower than model predictions in the zone above the heater, likely due to natural convection and buoyancy-driven vapor flow. If vapor transfer occurs during the duration of the elevated temperatures, then the bentonite may not fully hydrate, and thermal pressurization may not occur. This provides a motivation for having a well-calibrated and fully-coupled THM model with site-specific hydro-mechanical boundary conditions.
5. The importance of the magnitude of the bentonite swell pressure to the safety case of the engineered barrier system should be clarified. The magnitude of the bentonite swell pressure will depend on the initial density and initial suction before hydration and may change if the bentonite undergoes plastic thermal volume changes during the heating process. It may be useful to define a minimum swell pressure to ensure safety.
6. The magnitudes of thermal pressurization in the saturated bentonite buffer from long-term simulations by DOE have not been validated with experimental data. The estimated magnitudes appear to be quite high compared with experimental tests on the undrained heating of saturated low-plasticity clays in the literature (e.g., Ghaaowd et al. 2017), although it is acknowledged that data on thermal pressurization of bentonite is not widely available in the literature.
7. Although it has not been observed in the international field-scale experiments, desiccation cracking in compacted bentonite surrounding a heater is a potential phenomenon that should be studied as it may create preferential pathways for water or gas flow. It is possible that the stress state in the unsaturated, partially-hydrated bentonite may be sufficient to resist cracking during thermally-induced drying. However, bentonite desiccation is a phenomenon that may occur under the higher temperatures expected in the HotBENT experiments.
8. In the case that desiccation or other structural change occurs in the compacted bentonite during heating, it would be useful to study how thick a possible “sacrificial” zone near the heater or near other interfaces (i.e., the bentonite-shotcrete interface) should be to ensure long-term safety. This may be a useful topic to study in the context of the container failure at large times when the bentonite saturates.
9. Gas breakthrough through saturated bentonite is a complex problem and deserves further simulations and experiments for different stress/displacement boundary conditions. Specifically, it should be ensured that the stress/displacement boundary conditions in the experiments represent those expected in the engineered barrier system in the repository. In the laboratory experiments of Tomayo-Mas et al. (2018), the total stresses are applied in displacement-control conditions (i.e., due to the radial swelling of the bentonite and the axial stress applied by the end caps). When the gas pressure at the boundary increased to a

point that it was equal to the total stress (a point where the effective stress should be zero), the total stress increased with the gas pressure before gas breakthrough occurred (perhaps by hydraulic fracturing). If stress-controlled boundary conditions were to have been applied to the cell, shear failure may have occurred in the soil at a much lower gas pressure than observed in the experiment.

10. Details of the simulation of the gas breakthrough experiments are also not transparent. The evolution in total stress wasn't shown in the simulation results, so it is not clear if the changes in this variable were captured in the model. It was puzzling that the pore pressures along the length of the specimen did not increase proportionally to the gas pressure applied to the boundary but instead increased quickly after breakthrough. It seems that the water backpressure was applied to opposite side of the specimen during gas pressure application, and a gradual change in pore pressure would be expected along the length of the specimen. It was also not clear how the mean effective stress (used in the permeability function for the aggregate boundaries) was defined in the case that there are displacement-controlled total stresses, water backpressure, and gas pressure (i.e., a Bishop type effective stress used that considers the capillary pressure?).

Overall, it is my opinion the DOE researchers are making excellent use of available data from international underground laboratories to evaluate their modeling capabilities, and my feedback is intended to provide constructive suggestions on how to refine simulation capabilities to better capture the complex, coupled thermo-hydro-mechanical processes in engineered barrier systems in underground rock repositories.

Sincerely,

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