Developing constitutive relationships for the properties of unsaturated bentonite buffers under high temperatures

PI and Co-PI: John McCartney and Jiun-Shyan Chen, UCSD, La Jolla CA

Collaborators: LianGe Zheng and Hao Xu, LBNL, Berkeley CA

Program: FC-4.1: FC-4.1: Spent Fuel and Waste Disposition: Disposal

ABSTRACT:

The objectives of this project are to characterize the effects of high temperatures (up to 200 °C) on the mechanisms and material properties governing coupled heat transfer, water flow, and volume change in unsaturated, compacted granular bentonite, and to understand and simulate the multiphase hydration process of bentonite buffers in deep geological repositories with closely spaced waste packages or Dual Purpose Containers. The project tasks will include a combination of element-scale testing to measure bentonite material properties under high temperatures, tank-scale testing to capture the coupled processes during bentonite hydration under high temperatures, development of quantitative relationships to represent the experimentally-observed thermo-hydro-mechanical behavior, and numerical simulations of bentonite buffer hydration involving high temperatures for different initial densities and rates of water supply from the host rock. In the element-scale tests, different thermo-hydro-mechanical paths will be applied to compacted bentonite specimens having different initial conditions (density and degree of saturation) in thermal triaxial cells to collect data needed to define the new constitutive relationships. Specifically, these tests will investigate the impact of high temperatures and coupling between the soil-water retention curve (SWRC), hydraulic conductivity function (HCF), thermal conductivity function (TCF), volumetric heat capacity function (VHCF), thermo-elasto-plastic model parameters governing volume change during hydration/drying or heating/cooling, and properties governing nonequilibrium water phase change and enhanced water vapor diffusion. In the tank-scale tests, heat transfer and water flow processes in unsaturated bentonite will be monitored using an array of sensors during operation of a central heating probe and hydration from the boundaries to evaluate and refine mechanisms for nonequilibrium phase change and enhanced vapor diffusion in unsaturated deformable soils. A new SWRC model for deformable soils under high temperatures will be developed that separately accounts for water retained by adsorptive and capillary forces, which will also be used to define the effective stress state and couplings with other thermo-hydraulic properties of unsaturated deformable soils. An effective stress-based thermo-elasto-plastic model for unsaturated deformable soils under high temperatures will be developed with suction- and temperature-dependent yield limits to capture possible transitions from recoverable expansion to permanent contraction of overconsolidated bentonites under high temperatures. The new mechanisms and material properties will be implemented into COMSOL and TOUGH-FLAC to perform coupled heat transfer and water flow simulations of long-term bentonite buffer hydration under high waste temperatures and to investigate the role of different initial conditions (compaction conditions, use of artificial hydration, etc.) and impacts on the host rock excavation damage zone. An alternate approach involving physics-based and data-driven simulations within an in-house code at UCSD (NMAP) will also be developed using the experimental results that may be more efficient at considering the highly coupled processes. Deliverables will include coupled thermo-hydraulic relationships (SWRC, HCF, TCF, VHCF) for bentonite under high temperatures, a thermo-elasto-plastic constitutive model for unsaturated soils under high temperatures, new mechanisms for enhanced vapor diffusion and nonequilibrium phase change in unsaturated soils under high temperatures, and inter-code comparisons of long-term bentonite buffer hydration under high temperatures.