Goldschmidt 2022 Abstract
https://doi.org/10.46427/gold2022.11387

Effects of Temperature on the Thermo-Hydro-Mechanical Properties of Water-Saturated Compacted Clay

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Bentonite clay, a fine-grained geologic material rich in smectite clay minerals, is widely used in the isolation of landfills and contaminated sites and is considered for use as an engineered barrier in the disposal of high-level radioactive waste because of its unique properties, such as low hydraulic permeability and high swelling pressure. The heat released by nuclear waste is expected to exert large thermal gradients on this engineered clay barrier and may trigger coupled thermal-hydrologic-mechanical-chemical (THMC) phenomena that must be considered in the design of geologic repositories. Various material properties of bentonite clay are used as input in large-scale THMC simulators. A key requirement for achieving more accurate predictions of the performance of clay barriers is the establishment of more detailed knowledge of these material properties over a range of temperatures in a multi-physics system.

Here, we present a methodology that aims to generate new insight into the material properties of compacted bentonite using large-scale all-atom molecular dynamic (MD) simulations of clay-water mixtures carried out using the code GROMACS. The clay assemblage contains 27 Na-smectite particles with full atomistic-level resolution and is solvated using 187,131 water molecules (Fig.1). We generate 96 replicas of the system with exponentially increasing temperature and apply the replica-exchange MD (REMD) technique to facilitate the equilibration of the simulated systems. The simulations examine the impact of temperature (up to 100 °C) on the THMC properties of bentonite clay, including thermal conductivity, thermal expansion, heat capacity, hydraulic permeability, water/ion diffusivity, and swelling pressure. The results show that temperature increase induces a sequence of reversible and irreversible reactions in clay and alters the capacity of clay barriers to transfer heat, fluids, chemical species, and pressure. The constitutive relations obtained are then validated against existing experimental datasets on the material properties of bentonite.

The presented microscale THMC properties of bentonite buffer materials yield key inputs used in large-scale THMC simulators and enable comparisons with results at multiple scales. Finally, this work will facilitate characterization of clay evolution, help evaluate the performance of engineered clay barrier systems, and provide assurance for the long-term isolation of radioactive waste in geologic repositories.