

## An integrated multiscale experimental-numerical analysis on reconsolidation of salt-clay mixture for disposal of heat-generating waste.

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## **ABSTRACT:**

We propose a combined multiscale experimental and computational study to improve understanding of the thermal-mechanical-hydrologic-chemical (TMHC) coupling effect on the reconsolidation of granular (or crushed) salt-clay mixture used for seal systems of shafts and drifts in salt repositories. Our objective is to understand, in two phases how clay and moisture content affect the performance of backfill materials in the short and long term. In the first phase, microstructural experimental studies using a combination of micro-CT and SEM imaging techniques will help capture the geometrical features of reconsolidated salt/clay mixtures. These observations will be used to create realizations of microstructures for grain-scale polyhedral discrete element-lattice Boltzmann method (DEM-LBM) simulations. In the second phase, a new hierarchical discrete-to- continuum model will be utilized to convert pore-scale information (e.g. force exerted on grain boundary, sliding, pressure-solution) to continuum measures (e.g. Cauchy stress, Darcy's flow) at the integration points of the continuum model. Without using any macroscopic constitutive law, the resultant model can conduct 3D field-scale simulations by directly upscaling the interactions among the salt crystal, clay and moisture constituents without exhausting computational resources. This important feature will enable unprecedented predictions of the microstructural evolution of the clay-salt mixture while simulating field-scale events, such as brine intrusion and heat transfer between the salt and surrounding rock after the placement of hot waste. After calibrations, the DEM-FEM simulation results will help narrow down the clay and moisture contents that lead to optimal performance for the backfills. A number of macroscopic creep tests will then be used to further calibrate the numerical models and validate the multiscale predictions, with special emphasis placed on reconsolidation of very low porosities and at elevated temperatures.

The research will provide important experimental data analysis of the water absorption of the salt-clay mixture and how it affects the migration inclusion encountered along grain boundaries and micro-fractures at the early stage of repository. As a result, the proposed work will bring new insight into the sealing capacity of salt-clay mixture under elevated temperatures over a long period of time — a key to evaluating the potential of salt-clay mixture usage for salt repositories. Information obtained from this research will help engineers and repository scientists to design safer and more efficient seal systems. In particular, documentation will be accumulated in a stage-wise fashion and the research results will be published in archived journals and internal reports. The software and experimental data produced from this research will be made available for future benchmark and research purposes. The new collaboration between university and national Laboratories will provide valuable training to a new generations of graduate students, postdoctoral and undergraduate researchers with diverse research backgrounds. The research will provide valuable data and multiscale modeling capacity to enhance the performance and safety of heat-generating repository.