Development of Full Understanding of Mechanical-Chemical Coupling in Bentonite THMC Processes

PI: Cheng Chen, Virginia Tech

Collaborators: Yifeng Wang, Sandia National Laboratories

Program: Fuel Cycle

ABSTRACT:

Studies showed that the stress increase in an engineered bentonite clay barrier, resulting from lithostatic pressure, clay swelling, poro-elastic stress change, and thermal expansion, can exceed 1000 psi. Our central hypothesis is that this huge stress increase can lead to pressure solution (i.e., mineral dissolution at grain contacts) of sand, carbonates, and other minerals in the engineered barrier, which is the primary mechanical-chemical (MC) coupling mechanism in the engineered barrier and can lead to noticeable changes in pore water chemistry. Based on our previous experimental findings, the central rationale and motivation is that it is critical to eliminate the influence of dead-volume water in order to accurately characterize pore water chemistry in compacted bentonite clay in the laboratory. Based on this, the overall objective of this project is to develop full understanding of MC coupling in the thermal-hydrological-mechanical-chemical (THMC) couplings in the engineered barrier and its role on the development of large-scale barrier heterogeneity. Specific research objectives are: i) develop advanced laboratory experimental equipment and an improved clay dehydration model to enhance the accuracy of pore water chemistry characterization in bentonite clay under the influence of MC coupling (Aim R1); ii) use well-controlled laboratory experiments and a positive-feedback-based numerical model to unravel the role of pressure solution on the development of large-scale heterogeneity in an engineered barrier (Aim R2); and iii) develop advanced deep learning models, based on the convolutional neural network (CNN) and generative adversarial network (GAN), to obtain constitutive correlations between pore structure and hydrological transport properties and to obtain large-scale porosity oscillations that can be used in long-term performance assessments through THMC simulations (Aim R3). Despite many studies on TC, HC, TM, and HM couplings, a significant knowledge gap still remains in understanding the MC coupling, which regulates mineral stability and pore water chemistry. This project aims to develop full understanding of the role of pressure solution on pore water chemistry (Aim R1) and the implications to large-scale heterogeneity (Aim R2) and THMC processes (Aim R3) in engineered barriers. The research findings in this project will have practical applications to geologic disposal of high-level nuclear waste because pore water chemistry directly determines bentonite clay stability, longevity of the waste pack, and dissolution and migration of nuclides in the engineered barrier.