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Clay Hydration, Drying, and Cracking in Nuclear Waste Repositories

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Program: Fuel Cycle Technologies

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ABSTRACT:

This work will establish a new large-scale simulator for engineered clay barriers in the near field of a geological repository for high-level nuclear waste and spent nuclear fuel. This simulator will predict complex phenomena including barrier rehydration, fracture propagation and self-healing, and osmotic effects. It will incorporate detailed new knowledge of bentonite material properties on the molecular to particle scales and at temperatures up to 200 °C. It will be benchmarked against legacy and new experimental results on the performance of engineered clay barriers, including experiments carried out at underground research laboratories.

The project includes three major tasks. Task 1 will leverage computational fluid dynamics (CFD) simulation methodologies recently developed by the PI to develop a new large-scale simulator that can predict rehydration, cracking, and healing in engineered clay barriers. Task 2 will use all-atom and coarse-grained molecular dynamics (MD) simulations pioneered by the PI to constrain constitutive relations for the microscale properties of compacted clay used as input to the large-scale simulator. Task 3 will validate and refine the new large-scale simulator through benchmarking against core- and field-scale experimental results, including new results obtained as part of this project. The main deliverables are (*i*) progress reports every 6 months, (*ii*) annual and final project reports, (*iii*) reports for each milestone, (*iv*) peer-reviewed publications, and (*v*) a toolkit for the implementation of the new simulator in the free CFD solver OpenFOAM.

Key outcomes of the proposed work will be the development of (*a*) a new simulator for engineered clay barriers in high level waste and spent nuclear fuel repositories based on theoretical approaches in soft matter physics that can predict fracture propagation and healing in compacted clay, (*b*) new knowledge of the microscale properties of the compacted clay buffer material (particularly at temperatures up to 200 °C and for complex rheological properties) and associated constitutive relations that represent key input to large scale simulators, and (*c*) new experimental characterization of compacted clay properties (permeability, swelling pressure) and of fracture propagation and healing in compacted clay at elevated temperatures. The combination of these three outcomes will establish a new tested capability for large scale simulations of barrier evolution directly informed by molecular scale predictions of buffer material properties. This new multi-scale simulation capability will enable robust cross-comparisons with experimental results at multiple scales. These developments will increase confidence in the robustness of generic disposal concepts, help identify sources of uncertainty in these concepts, provide a sound technical basis for the evaluation of multiple viable disposal options, and unlock future advances in buffer material by design.