

Radionuclide Waste Disposal: Development of Multi-scale Experimental and Modeling Capabilities *University-Led Research*

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This project is a Department of Energy, Experimental Program to Stimulate Competitive Research (EPSCoR) Implementation Grant. The experimental and modeling efforts of this project are guided by the overarching scientific question:

What are the major molecular level chemical, biological, and microbial interactions that control the mobility of radionuclides in natural and engineered systems and how can these molecular and pore scale processes be properly defined and quantified for incorporation into larger scale, coupled experimental systems and reactive transport modeling efforts?

The key issues to be addressed include identifying source terms for contaminants in geologic disposal scenarios, determining the chemical speciation of risk-driving radionuclides (*e.g.*, Np, Tc, Cs, U, I) within engineered waste forms and natural subsurface environments, delineating the biogeochemical and physical processes through which contaminant transport is manifested, and predicting contaminant mobility across wide temporal and spatial scales. The project is undertaken by an interdisciplinary team from three South Carolina universities. The project is divided into four major tasks as well as the development of a new imaging facility capable of monitoring the 2D and 3D transport of radionuclides through engineered waste forms and natural soils.

Major accomplishments of the project to date include:

- Testing of Single Photon Emission Computed Tomography (SPECT) imaging systems using a column with an idealized soil structure.
- Design and groundbreaking on a field lysimeter facility used to monitor transport of U, Tc, Np, I, and Cs under natural conditions.
- Experimental and quantum-mechanical modeling studies of hollandite compositions of the form $Ba_xCs_{2.32-2x}Ga_{2.32}Ti_{5.68}O_{16}$ are underway with varying A site (Ba/Cs) composition.
- Characterization of Tc behavior in reducing grout/cementitious waste forms under controlled laboratory and field conditions have examined the rate of Tc(IV) oxidation to Tc_2S_7 and TcO_4^- . Complimentary studies are underway to examine the use of graphitic nanoreinforcements to alter strength and porosity of the waste form.
- Component additivity surface complexation models describing Tc, U, and Cs sorption to a Savannah River Site sandy loam soil have been developed.
- A kinetic model describing competitive ion sorption processes has been developed which can account for competition between weakly and strongly sorbing ions across a wide range of concentrations. A kinetic rather than equilibrium model is needed to account for the expected disequilibrium within pore waters.