Upscaling of U(VI) Desorption and Transport from Decimeter-Scale Heterogeneity to Plume-Scale Modeling

Federal Agency-Led Research

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Applications of reactive transport modeling of contaminants in groundwater can often be limited by because experimental data are available at the centimeter scale but field-scale transport occurs on the kilometer scale. The focus of this project is to test approaches for defensibly incorporating small-scale information into field-scale simulations. The project is using extensive previously collected datasets at bench-, decimeter-, and tracer-test scales to support field-scale simulations of uranium transport in the shallow alluvial aquifer at the Naturita, Colorado UMTRA site. The decimeter scale experiments were conducted in 2 dimension tanks that provide a unique opportunity to impose chemical gradients in experiments with known heterogeneity. U(VI) adsorption was simulated using both one-site and two-site models which were calibrated to batch desorption data for three size fractions. These surface complexation models were then incorporated into multicontinuum mass-transfer models which were successfully calibrated to column, decimeter-scale and tracer test experimental results. High-resolution simulations of two new 2D tank experiments that have incorporated the bench-scale models have been conducted. Two 2D tank experiments will be conducted simultaneously based on the results of the high-resolutions simulations. The size of the tanks will be 2.4 m x 1.2 m x 7.6 cm and 2.4 m x 0.6 m x 7.6 cm.

Two tracer tests were conducted in the summer and fall of 2011 to observe *in situ* desorption processes over longer time scales compared with previous experiments. Whereas both tests were monitored by conventional groundwater sampling, the fall 2011 test was also monitored using time-lapse electrical resistivity tomography between two rows of down-hole electrodes augmented by several surface electrode arrays. Preliminary analysis of the combined time-lapse resistivity and geochemical sampling data provide insights into the spatial-temporal evolution of the tracer across the site. Work is ongoing to compare the geophysical and geochemical results to evaluate mass transfer and identify preferential flowpaths.

A combined analysis of data from these laboratory experiments and field tracer tests will be used to evaluate upscaling approaches at two distances from the injection gallery. Knowledge of the spatial distribution of sedimentary facies defined by previous geophysics studies, coupled with new sediment acquisition and characterization, will provide a better understanding of heterogeneity at the plume scale. Ultimately, plume-scale predictions of U(VI) transport for 13 years (1999-2012) will be compared with measured values in the aquifer, with upscaling of reactive transport parameters in accordance with the meter-scale studies.