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

ABSTRACT: Modeling reactive transport of contaminants in groundwater is uncertain because detailed experimental laboratory data are available at the centimeter scale but field-scale transport occurs on the kilometer scale. In this project we test approaches for incorporating small-scale information into field-scale simulations using extensive datasets collected at bench-, decimeter, and tracer test scales of U(VI) at the Naturita, Colorado UMTRA site.

Laboratory batch experiments using contaminated sediments from the Naturita site indicated that U(VI) desorption was rate-limited and required on the order of 30 days to reach equilibrium. Simulations using a dual domain mass transfer model indicated that after approximately 2 weeks the temporal changes of the U(VI) concentration were driven by weathering reactions. The decimeter scale experiments were conducted in 2.5m long 2D tanks packed with two size fractions excavated from the field site. Desorption of U(VI) was simulated using an equilibrium surface complexation model calibrated to batch data and mass transfer rate parameters estimated by model calibration. Reactive transport in the more permeable fraction was limited by the desorption rate whereas equilibrium was closely approximated in the less permeable material. These results were extended in synthetic upscaling experiments where a 2D domain was successfully simulated by a 1D dual domain model using immobile porosity values estimated from the volume fraction of the less permeable facies.

Analysis and modeling of two tracer tests conducted at the Naturita field site has further demonstrated importance of rate-limited mass-transfer on U(VI) transport. Electrical resistivity measurements used to monitor a tracer experiment that had a high sodium chloride concentration demonstrated that effective parameters for mobile-immobile zone transfer could be determined both along the flowpath as well as locally at an observation well, providing insight into the spatial variability of the mass transfer processes. Results from these studies were extended to simulate U(VI) transport observed in the second tracer test where a low electrical conductivity, U(VI) free water was injected into the aquifer. The results demonstrated that the model calibrated to electrical observations coupled with U(VI) surface complexation model developed in the laboratory had significant predictive capability of field transport. A combined analysis of data from the laboratory experiments and field tracer tests is being used to evaluate upscaling approaches at the plume scale. Ultimately, plume-scale predictions of U(VI) transport for 16 years (1998-2013) will be compared with measured values in the aquifer, with upscaling of reactive transport parameters in accordance with the meter-scale studies.