Simulating U(VI) desorption and transport from decimeter-scale experiments to the plume-scale

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Reactive transport simulations offer the potential of predicting the long term fate of contaminants such as uranium in groundwater aquifers. This capability may lead to better site management and a transparent assessment of contaminant fate, transport and risk. However, applications of reactive transport modeling in groundwater can be limited because experimental data are often available at the centimeter scale whereas field scale transport typically occurs on the kilometer scale. To bridge this gap, hexavalent uranium (U(VI)) desorption rates were investigated across multiple scales including batch, column, 2m intermediate scale lab experiments and 1-4m tracer test experiments in order to more accurately describe transport at plume scale. At the batch scale, U(VI) desorption was rate-limited and characterized by an initial rapid increase in U(VI) concentration in the first 400 h followed by as slow release for up to 2000 h. Simulations using a multirate mass transfer model to describe U(VI) desorption indicated that after 400 h the temporal changes of the U(VI) were driven by weathering reactions rather than slow desorption. Simulations of column experiments with sediments from the field site showed significant concentration rebound when flow was interupted and the extent of rebound was sensitive to alkalinity. Rebound observed in intermediate scale (~2 m) lab experiments decreased with distance because the concentration gradient between the mobile and immobile zones decreased along the flowpath. Tracer tests conducted in the field were monitored by both a geoelectrical resistivity network and groundwater sampling and demonstrated importance of rate-limited mass-transfer on U(VI) transport. A reactive transport model that coupled mass transfer with U(VI) surface complexation model had significant predictive capability of the field transport. These results will be used in a post audit of a reactive transport model calibrated to field data from 1986-2001 and to compare predictions with data collected regularly since 2002.