Field-scale Estimation and Simulation of Biogeochemical Heterogeneity

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Many bioremediation experiments have been conducted at the DOE Rifle (CO) IFRC site to facilitate the reduction of U(VI) to U(IV) and to explore the role of the associated coupled physical and biogeochemical processes. At the Rifle IFRC and elsewhere, it is common to use time-lapse wellbore-based aqueous geochemical data with mechanistic models to assess the progress of the remediation-induced system transformations. In this work, we strive to identify the diagnostic signatures of biostimulation by using hydrological, geochemical, and geophysical data through two different yet complementary approaches.

In the first study, we use a data-driven statistical (or 'top-down') approach to identify system transformations that occur during bioremediation using time-lapse aqueous geochemical data (such as Fe(II), sulfate, sulfide, acetate, and uranium concentrations) and spectral induced polarization (SIP) data. We consider the multivariate geochemical concentrations as hidden random processes (observed at borehole locations but unknown at other locations) and the time-lapse geophysical data as observations at each location along the 2D profiles. The connection between the geophysical observations and geochemical time-series is determined by design matrices that depend upon redox status. We use a Bayesian approach to estimate the unknown parameters and use Markov chain Monte Carlo methods to draw many samples from the joint posterior distribution. We find that the developed statistical approach can provide information about (1) the probability of being in each redox stage over time and space following biostimulation, and (2) diagnostic parameters as functions of aqueous geochemical concentrations and geophysical attributes. The top-down approach is expected to be especially useful for rapid identification of critical system transitions based on streaming monitoring data and for constraining mechanistic transport models where various reaction pathways are possible.

In the second study, we use a mechanistic reactive transport modeling (or 'bottom-up') approach to combine hydrological, geophysical, and geochemical data. We use flowmeter and slug test data to set up the initial distribution of permeability. The initial distribution of porosity was obtained by assuming a correlation between porosity and permeability and by matching bromide breakthrough data and SIP data at the initial time. We use inverse reactive transport modeling of time-lapse geochemical data to determine key parameters that control the reactive transport processes. After obtaining a good match with the geochemical data, we compare the predicted aqueous and solid phase geochemistry from the reactive transport model with the SIP data to understand key controls on the SIP data and whether the SIP data are useful for monitoring and diagnosing changes in the biogeochemical processes during the biostimulation experiments. The established method can be used to link geochemical and geophysical signatures and eventually to help understand and predict subsurface biogeochemical processes using constraints from different types of measurements. This mechanistic approach is complementary to the data-driven, statistical approach in that it allows us to gain a better understanding of the key controls on overall system behavior.