UNCERTAINTY QUALIFICATION OF BIOGEOCHEMICAL MODELS FOR ETHANOL-STIMULATED URANIUM (VI) REDUCTION IN SUBSURFACE SEDIMENTS

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In situ bioremediation of a uranium-contaminated aquifer with different electron donors, including ethanol, acetate and emulsified vegetable oil (EVO) has been tested at the US DOE Subsurface Biogeochemical Research Program (SBR) Integrated Field Research Challenge (IFRC) site, in Oak Ridge, TN. Many biogeochemical models have been developed to describe the coupled processes involved in the reduction of soluble uranium (VI) to sparingly soluble and immobile U(IV). However, not enough attention is given to the prediction uncertainty caused by the uncertainty from the model structures and many input parameters. In this study, we first implemented a physiology-based biogeochemical model [Istok et al., 2010; Jin and Roden, 2011] with the geochemical modeling program PHREEQC. This model was applied to the results of laboratory microcosm tests examining the effect of initial sulfate concentrations (1 versus 4 mM) using ethanol as electron donor. We used time-dependent concentration profiles for sulfate, acetate and uranium to calibrate model parameters. Global sensitivity analysis approach was subsequently performed to identify the important parameters affecting the objective function defined by the sum of square weighted residual between observation and simulation concentration; the objective function is used to carry out parametric uncertainty assessment using the Markov Chain Monte Carlo (MCMC) methods in a subsequent step. A recently developed MCMC-based approach, DiffeRential Evolution Adaptive Metropolis (DREAM), is applied to quantify the posterior parameter distributions. Another laboratory experiment data set, reported by Mohanty et al. [2008] and Jin and Roden [2011], is used to assess predictability through Bayesian credible intervals. This study is focused on parametric uncertainty, which allows us to understand the biological and geochemical processes in more detail and to improve accuracy of model prediction. The model uncertainty from different conceptualizations and/or mathematical descriptions of redox reactions will be analyzed in the near future.