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ABSTRACT TITLE: Multiscale Assessment of Prediction Uncertainty in Coupled Reactive Transport Models

ABSTRACT: Reactive transport simulations provide a systematic framework for integrating hydrologic and biogeochemical conceptual process models into a quantitative description of subsurface behaviors, which can then be used to project future concentrations. Assessing the uncertainty of these projections is difficult, because subsurface environments are open and complex, and subject to multiple interpretations and conceptualizations. This challenge is addressed using the method of multimodel analysis, in which model predictions are based on a weighted average of predictions of multiple plausible models, each of which is associated with a model averaging weight estimated from a maximum likelihood Bayesian model averaging approach.

The model averaging approach was evaluated for uranium transport at the Naturita UMTRA site using available data at the batch, column and tracer-test scale and in synthetic 3D simulations at the plume scale. At the batch and column scales, significant uncertainty results from imperfect knowledge of the adsorption reactions that immobilize uranium at the mineral surfaces as well as auxiliary reactions such as speciation and ion exchange. At the tracer test scale and especially in the 3D plume scale, additional uncertainty results from imperfect knowledge of the distribution of the reactive facies that describe the flow, transport and reactions. Model averaging had superior predictive coverage in both the column and tracer test analyses. The results for the synthetic physically and geochemically heterogeneous 3D study showed little support for oversimplified models such as those with homogeneous layers or zonal distributions of reactive facies. Heterogeneous distributions of reactive hydrofacies generally performed well; in some but not all instances these models gave superior predictions relative to model averaging. Model averaging had superior predictive coverage by considering model uncertainty. Parametric and conceptual model uncertainty for the stimulated bioreduction of U(VI) by microbial processes at the Rifle IFRC site was evaluated using a set of synthetic observations generated by a 3D reactive transport simulation of the Big Rusty field experiment. The ability to parameterize a comprehensive reaction network using a 1D model of the simulated 3D system was evaluated using sensitivity analysis and parameter estimation methods. Evaluation of the 1D approach was based on the ability of the calibration to estimate the known parameter values used in the 3D simulation, and on the suitability of the resulting parameter uncertainty estimates used in assessing predictive uncertainty. Results indicated that, although the 1D model can provide concentrations of key constituents that are representative of the 3D system, spatial variability in groundwater flow that is unresolved in the 1D abstraction can significantly bias the estimated reaction parameters. Derived linear parameter uncertainty estimates tended to be much smaller than indicated by the known conceptual errors. Without considering the impact of these conceptual errors, predictive uncertainty could be significantly underestimated.