Computational Bayesian Framework for Quantification and Reduction of Predictive Uncertainty in Groundwater Reactive Transport Modeling

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Subsurface environmental systems are open and complex, in which intricate bio-hydro-geochemical processes interact across multiple spatial and temporal scales. Predictions of the subsurface system are inherently uncertain, and uncertainty is one of the greatest obstacles in groundwater reactive transport modeling. The goal of this project is two-fold: (1) developing new computational and mathematical methods for quantification of predictive uncertainty, and (2) using the developed methods as the basis to develop new methods of experimental design and data collection for reduction of predictive uncertainty.

In the second year of the project, we have developed a computational Bayesian framework for uncertainty quantification. The framework considers various sources of uncertainty in data, model structures, model parameters, and driving forces (e.g., natural changes related to climate change and human-induced engineering remediation). The framework can be used to evaluate predictive uncertainty from these sources and to identify major uncertainty sources. Based on this framework, we have extended variance-decomposition-based sensitivity analysis from a single model/scenario to the context of multi-models/scenarios. This is necessary to reliable selection of influencing model parameters and components, because parameter sensitivity may vary between models and/or scenarios. The Bayesian framework has been evaluated using a synthetic modeling that considers three scenarios of precipitation (due to climate change), two models that convert precipitation to recharge, and four parameters of groundwater flow and reactive transport. We have demonstrated that a large amount of computational cost can be saved by using the sparse-grid methods to implement numerical calculation of the framework. The framework will be used for the rest of the project for uncertainty quantification and reduction.

A number of insights have been gained through our numerical analysis for groundwater reactive transport modeling. We have shown that model residuals are non-Gaussian due to nonlinearity of biogeochemical reactions and coupling of flow, transport, and reaction processes. Using a more appropriate likelihood function can improve model prediction to reduce biasness in predictions and yield more accurate uncertainty quantification. For surface complexation models of uranium adsorption, we demonstrated that parametric uncertainty is caused by competing effects between different functional groups and between different reactions on a single functional group. This finding leads to the conclusion that effective and efficient uncertainty reduction can be achieved by designing column experiments that constrain the competing effects. In addition to the biogeochemical insights, we have also gained insights into numerical evaluation of marginal model likelihood function needed for quantification of model uncertainty.