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ABSTRACT TITLE: Improving the reactive transport modeling at the Hanford 300 Area with a Bayesian data assimilation framework

ABSTRACT: Data assimilation is an important tool to enhance the interactions between the field and lab experiments and system-scale model developments. The ultimate goals are to advance our understanding of the system and reduce the uncertainty in model predictions. We demonstrate a Bayesian data assimilation framework that can integrate information from different sources in a sequential manner, using the reactive transport modeling at the Hanford 300 Area as an example.

Flow and transport processes within the Hanford 300 Area are impacted by the extremely dynamic groundwater-riverwater exchange with the adjacent Columbia River and heterogeneous distribution of source terms within the site. To improve the accuracy of reactive transport modeling at the site, it is essential to reduce the hydrologic uncertainty (transient flow boundary conditions and the underlying heterogeneous hydraulic conductivity field) and geochemical uncertainty (geochemical reaction processes and parameters, and heterogeneity in initial uranium distributions). We reduced such uncertainties by assimilating multiple types of data obtained from various field experiments conducted at the Hanford 300 Area. In the hydrologic data assimilation step, data from constant-rate injection tests, borehole flowmeter profiling, and conservative tracer tests, are sequentially assimilated across scales using a combination of Bayesian techniques to reduce uncertainty in the estimated permeability field. The hydrologic data assimilation is then followed by geochemical data assimilation, where the goal is to infer the initial condition and geochemical parameters, such as sorption sites and reaction rates, by assimilating breakthrough curves of a reactive tracer observed during adsorption/desorption field experiments. The computational demand was managed by using the multi-realization capability within the parallel PFLOTRAN simulator. The Bayesian data assimilation framework has been shown to be efficient and effective in integrating multiple types of data for uncertainty reduction and improving model predictions.

The general data assimilation framework we developed in this study can be readily applied to integrate model developments and field experimental data in other complex systems at various scales. In future studies, we will apply this framework to study a coupled hydro-biogeochemical model (including C/N cycling and microbial community dynamics) in the dynamic groundwater-river water interaction zone in the Hanford 300 Area, integrating multiple types of spatio-temporal data, such as microbial community, geochemistry, hydrological and geophysical measurements, and others.