Hybrid Multiscale Simulation of Hydro-Biogeochemical Processes in the Groundwater-Surface Water Interaction Zone

PNNL SBR SFA (Laboratory Research Manager: Charlette Geffen)

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The PNNL SFA is developing a predictive understanding of the groundwater-surface water interaction zone (termed the subsurface interaction zone, SIZ). A key element of this research is a multiscale modeling framework that facilitates the integration of new mechanistic understanding from fine-scale controlled laboratory studies (bottom-up) with diverse field-scale observations (top-down). Our hybrid multiscale modeling approach couples models of fluid flow and biogeochemical transport formulated at various scales (e.g., pore, darcy, and field scales) to provide increased process fidelity when and where needed (according to well-defined model error criteria) while maintaining computational feasibility over a large domain. The SIZ plays an important role in natural ecosystems as it functions as an interface between terrestrial, subsurface and aquatic systems. Locally it regulates the mixing of nutrients that control biogeochemical transformations of solutes of both groundwater and riverine origin. Subsurface heterogeneity can give rise to local hotspots of microbial activity that are important to system function yet difficult to resolve computationally. To address this challenge, we are testing our hybrid multiscale approach using the same field-scale model domain utilized in SFA Task 2 field and modeling studies (Stegen et al. poster; Chen et al poster). The region of interest intersects the aquifer and the river and contains a contaminant plume. However, biogeochemical activity appears to be highest in a thin zone (river alluvium layer, <1 m thick) immediately underlying the river where organic matter accumulates. It is not computationally feasible to resolve the full macroscale domain at the fine resolution potentially needed in the alluvium layer, and the multi-component reaction network applicable in the alluvium layer is more complex than is needed in the rest of the macroscale domain. Hence, the hybrid multiscale approach is used to couple high-fidelity simulations of alluvium layer processes with coarsely-resolved simulations of the larger domain. Models at both scales are simulated using the PFLOTRAN code in a series of increasingly complex system conceptualizations: 1) Homogeneous alluvium and uniform biogeochemical reaction network (comparable to the Task 2 single-scale model); 2) Heterogeneous alluvium and uniform biogeochemical reaction network; and 3) Heterogeneous alluvium and more complex biogeochemical reaction network in alluvium layer. Through this series of numerical experiments, we are able to quantify the computational costs and differences in model predictions associated with the multiscale hybrid method, and to quantify the potential impacts of biogeochemical hotspots in the alluvium layer on system behavior.