

Resolving environment-microbe feedback at the pore scaling using a reactive transport model integrated with genome-enabled microbial metabolism

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Microbial processes mediate a variety of chemical transformation in subsurface environments. Their rates of reactions depend on local substrate availability, which may necessitate the flow and transport conditions at the pore scale to be resolved. Here we present our novel reactive transport model based on a Lattice-Boltzmann implementation of flow and transport equations which can take into account complex physical and geochemical feedbacks and enables massive parallelization that makes larger environmental simulations possible.

In reactive transport simulations, biochemical rates are often described with conventional rate expressions, such as Monod kinetics, which rely on ad hoc rate parameters. To take advantage of the vast growth of knowledge on microbial metabolism, our pore scale modeling framework is designed to utilize advances in genome-scale microbial metabolic reconstructions through the integration of flux balance models (FBM) capturing cell metabolism *in silico*. When employed across space and time, the numerical solution of coupled FBM–reactive transport models becomes computationally very expensive due to iterative implementations of linear programming in every time point and spatial grid. We address this through the use of surrogate models such as artificial neural network representations of microbial metabolic models. This confers substantial computational speed-up, which facilitates simulating complex microbial metabolic exchanges with surrounding environments. Our work therefore allows us to account for microbial processes in dynamic subsurface environments with unprecedented resolution, significantly increasing our ability to predict multi-scale, multi-physical biogeochemical and reactive transport dynamics.