High performance reactive transport simulation at the pore scale to investigate the effect of pore scale flow on average geochemical reaction rates

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Abstract
The scale-dependence of geochemical reaction rates hinders their use in continuum scale models intended for the prediction of chemical fate and transport in subsurface environments such as those considered for geologic sequestration of CO2. Processes that take place at the pore scale may contribute to the lab-field discrepancies commonly observed. Here, we investigate the dependence of mineral dissolution rates on the pore structure of the porous media using a novel pore scale modeling approach. The pore scale model is composed of high-performance tools and algorithms for direct simulation of incompressible flow (Navier-Stokes) and conservative transport (Chombo) combined with a multicomponent geochemical reaction code (Crunchflow). We addressed considerable technical challenges including modeling fluid-solid interactions on a structured grid, computational efficiency and parallel efficiency. A novel algebraic multigrid method (AMG), which automatically resolves the complex geometries, was found to perform much better than traditional geometric multigrid (GMG). Using the case of calcite dissolution as an example, the high-resolution model is used to demonstrate that nonuniformity in the flow field at the pore scale has the effect of decreasing the overall reactivity of the system, even when systems with identical reactive surface area are considered. The effect becomes more pronounced as the heterogeneity of the reactive grain packing increases, particularly where the flow slows sufficiently such that the solution approaches equilibrium locally and the average rate becomes transport-limited.