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High performance 3D simulation of reactive transport in porous media using level set method XIAOYI LI, Research Associate, Idaho National Laboratory, HAI HUANG, Research Scientist, Idaho National Laboratory, PAUL MEAKIN, Fellow Research Scientist, Idaho National Laboratory — The coupled processes of fluid flow, solute transport and mineral precipitation/dissolution in porous media are of great interest in a large variety of scientific and engineering areas. In this work, a high performance parallel simulator using MPI is developed to simulate pore-scale coupled reactive fluid flow and structure evolutions in porous media with complex and realistic pore geometries. Convection, diffusion, and chemical reaction resulting in geometrical changes in the pore spaces are treated simultaneously. The reaction-induced evolution of solid grain surface is captured using a level set method. A more elegant sub-grid representation of the interface is obtained by using the level set approach, instead of the pixel-based representation of the interface used in most lattice-Boltzmann and cellular-automata methods. The performance scaling of the method is demonstrated. The precipitation in a 3D random porous medium represented by packed solid spheres is simulated and discussed. More realistic relationships between permeability and porosity of the porous media are obtained from simulation. The simulation can provide a physics-based permeability-porosity model for continuum-scale reactive transport simulations.

Xiaoyi Li
Research Associate, Idaho National Laboratory

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