Level set simulation of precipitation and dissolution of flow-transported reactive solutes in porous media XIAOYI LI, HAI HUANG, PAUL MEAKIN, Center for Advanced Modeling and Simulation, Idaho National Laboratory — The coupled process of flow, transport and precipitation/dissolution of reactive solutes in porous media is important in a large variety of scientific and engineering areas. Examples include evolution of geological fractures, acid stimulation in petroleum recovery, and retardation of contaminant transport in groundwater.

In this work, we develop an innovative numerical tool to simulate reactive flow and structure evolution at the pore scale. Convection, diffusion, and chemical reaction resulting in changes in the pore space geometry are treated simultaneously by solving coupled momentum and solute transport equations. The reaction-induced evolution of solid grain surface is captured using a level set method. We obtain a more elegant sub-grid representation of the interface using a level set approach, instead of the pixel-based representation of the interface used in most lattice-Boltzman and cellular-automata methods. The model is validated against analytical solutions for simplified geometries. The patterns of precipitation/dissolution in a simple throat as well as a random porous matrix are discussed. The quantitative relationships among hydraulic properties (e.g. permeability and porosity) of the porous media are obtained from simulation. The results elucidate the underlying mechanism of the reaction-induced property changes in porous media.

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