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A numerical simulation method for dissolution in porous and fractured media. (English)

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Summary: We describe an algorithm for simulating reactive flows in porous media, in which the pore space is mapped explicitly. Chemical reactions at the solid-fluid boundaries lead to dissolution (or precipitation), which makes it necessary to track the movement of the solid-fluid interface during the course of the simulation. We have developed a robust algorithm for constructing a piecewise continuous (C_1) surface, which enables a rapid remapping of the surface to the grid lines. The key components of the physics are the Navier-Stokes equations for fluid flow in the pore space, the convection-diffusion equation to describe the transport of chemical species, and rate equations to model the chemical kinetics at the solid surfaces. A lattice-Boltzmann model was used to simulate fluid flow in the pore space, with linear interpolation at the solid boundaries. A finite-difference scheme for the concentration field was developed, taking derivatives along the direction of the local fluid velocity. When the flow is not aligned with the grid this leads to much more accurate convective fluxes and surface concentrations than a standard Cartesian template. A robust algorithm for the surface reaction rates has been implemented, avoiding instabilities when the surface is close to a grid point. We report numerical tests of different aspects of the algorithm and assess the overall convergence of the method.

MSC:

76S05 Flows in porous media; filtration; seepage
76M28 Particle methods and lattice-gas methods
76M20 Finite difference methods applied to problems in fluid mechanics

Keywords:

dissolution; porous media; lattice-Boltzmann; finite-difference

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NAG; nag

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