Geophysical Research Abstracts, Vol. 9, 05514, 2007
SRef-ID: 1607-7962/gra/EGU2007-A-05514

Multiscale model for reactive transport and mineral precipitation in porous media

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A new multiscale reactive transport model was developed and used to simulate the precipitation of solid phases from soluble precursors in systems with flow and mixing. The model was used to simulate the side-by-side injection of Na2CO3 and CaCl2 solutions into two halves of a three-dimensional granular porous medium. Subsequent mixing of the two solutions resulted in CaCO3 precipitation on grain surfaces along a narrow zone in the middle of the domain. The pore scale model was used to simulate solute mixing and mineral precipitation in this narrow zone while a continuum scale model was used to model the solute transport in the rest of the porous medium. The multiscale model is based on the Smoothed Particle Hydrodynamics (SPH). The meshless particle nature of SPH allows an easy coupling between pore and Darcy scales. Particle methods also allow complex physical and chemical processes to be incorporated into the model, through particle interactions, with relatively little code-development effort. The width of the precipitation zone was found to be practically independent of the Peclet number, Pe, but the precipitation rate increased with increasing Pe. The width of the mixing zone decreased with time as precipitated minerals filled pore space and reduced contact between the Na2CO3 and CaCl2 solutes. The large reduction in the mixing of the two solutes is a phenomenon that can not be accurately described by traditional Darcy scale models. The numerical simulations qualitatively reproduced the behavior observed in related laboratory experiments.