Lattice Boltzmann pore-scale model for coupled multi-component flow, diffusion, and reaction

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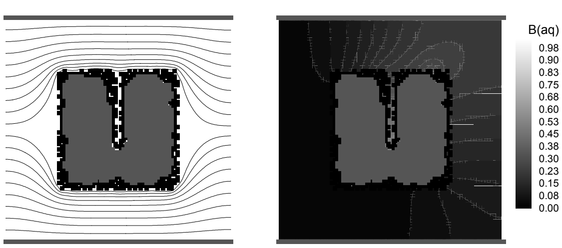
Numerical method

In this work, we present a multi-component lattice Boltzmann model for simulating reactive transport in porous media at the pore scale taking into account flow and diffusion in complex geometries. In the model, a set of distribution functions is introduced to simulate fluid flow and solute transport. The evolution equations recover the correct continuity and Navier-Stokes equations, and convection-diffusion-reaction equations [Kang et al., 2002].

This model takes into account convection, diffusion, homogeneous reactions among multiple aqueous species, heterogeneous reactions between the aqueous solution and minerals, as well as the resulting geometrical changes in pore space. Homogeneous reactions are described through local equilibrium mass action relations. Mineral reactions are treated kinetically through boundary conditions at the surface. We have applied this model to a variety of multi-component systems in synthetically constructed media, and analyzed the effects of convection, diffusion, reaction rate constants, equilibrium constants, and chemical compositions on mineral alteration of the porous medium.

Figure 1: Geometry, stream lines (left) and contours of solute B (right)



Discussion of results

Figure 1 shows the simulation results of a system with solute species A, B, C, and minerals AB (denoted as gray symbols) and AC (denoted as black symbols) undergoing reactions A+B=AB and A+C=AC. Initially, only AB exists in the domain in equilibrium with A and B. A solution including only A and C (in equilibrium with AC) is introduced at the entrance. Mineral AB dissoves, causing precipitation of AC.

Reference

Kang Q. *et al*. (2002) Phys. Rev. E, 66, 036318.

Bubble growth in soft sediments: Diffusion meets solid mechanics

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The quantitative description of diffusion and reaction with multiple physical phases presents significant challenges to both experimentalists and modellers; however, such problems arise naturally and commonly in geochemical systems. The growth of bubbles in soft organic-rich sediments offers a particularly striking example. Methane is generated in porewaters from the anoxic decomposition of organic matter, after the exhaustion of all inorganic oxidants. The resulting methane concentrations often exceed saturation with respect to the gas phase, and bubbles regularly form. An understanding of the formation of such bubbles is difficult to obtain: sediments are visually opaque, the bubbles are relatively small generally (1 cm^3 or less), and the slow growth rates complicate direct observation. In addition, the nature of the mechanical interaction between the growing bubble and the medium has been ignored, but it is crucial to the problem .

Recent advances in two experimental methods have shed considerable light on the mode of formation of these bubbles. The first is the development and application of high-resolution CT-scanning; such images have shown that bubbles in soft sediments are highly eccentric and distorted disks. The second methodology has been the development of a micro-injector system that can create bubbles in sediments and simultaneously measure their internal pressure. The information from these techniques indicates that bubbles grow by fracturing the adjacent sediment, not by fluidization as might be assumed.

Given this type of mechanical interaction between bubble and sediment, it is possible to create a reaction-diffusion-fracture model. Methane is generated by a distributed source in the sediment and moves by molecular diffusion to the bubble nucleation site (assumed abundant). The sediment responds as a linear-elastic solid to the increased gas concentration in the bubble until a critical stress is achieved, at which time the sediment fractures instantaneously and the bubble elongates a finite distance. This process is repeated to create a bubble that becomes more eccentric with size/time. The shape predictions of this model are completely in accord with the CT and injection data and predict growth times on the order of days for an organic-rich site in the USA.

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