Particle tracking numerical methods for nanoparticle transport in heterogeneous porous media

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ABSTRACT

A single-phase flow, lattice Boltzmann method (LBM)is utilized with a Lagrangian particle tracking (LPT) method for the simulation of flow and transport of nanoparticles in a porous medium. The 3D pore matrix is obtained either as a randomly packed with spheres porous medium or from images of segments of rock (sandstone) through micro-computed tomography (micro-CT).

The flow of a Newtonian fluid passing through this digital porous matrix is obtained with the LBM. A large number (on the order of 10,000 – 100,000) of Lagrangian markers that designate the motion of nanoparticles are injected in the flow field and are then numerically followed in time and space. We simulate the motion of the nanoparticles using an equation of motion that takes into account convection and random Brownian motion. The concentration of the particles is very low, so that the particles can be assumed to be passive [1]. When the particles collide with the solid matrix, they can either adsorb or continue their motion, based on the assumption that the deposition process is a pseudo-first order process. Furthermore, the solid-fluid interface is assumed to be heterogeneous, so that the simulated nanoparticles can adsorb at different rates at different sites of the interface. In our simulations, we use four different types of adsorption sites, in correspondence to the four major minerals composing sandstone. We validate the simulations with theoretically expected results, based on macroscopic filtration equations, and with experiments contacted by our collaborators at the University of Oklahoma and with experiments available in the literature [2].

Prior experimental work has shown that the pattern of pore surface heterogeneity does not much affect particle deposition [3]. Our work indicates that there are conditions for which the pattern of heterogeneity can be important in deposition. These are conditions on molecular diffusivity of the particles (the Schmidt number of the particles), nominal deposition rate (the Damkohler number) and flow conditions (the Peclet number). A range of particles with Schmidt numbers spanning orders of magnitude (up to Sc = 21500) have been simulated. The presentation will include a description of the LBM/LPT numerical approach, the validation of the technique, and results for porous media with different heterogeneity patterns.

REFERENCES

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