Development of Enhanced 3D Simulation Capability for Analyzing Migration of Colloids in Complex Flow Domains

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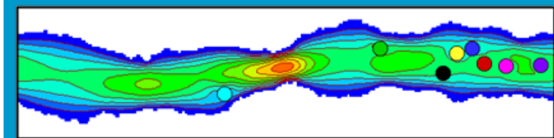

Fig. 1. Particles flowing in a fracture channel with fractal surfaces. Contours represent flow velocity (model result).

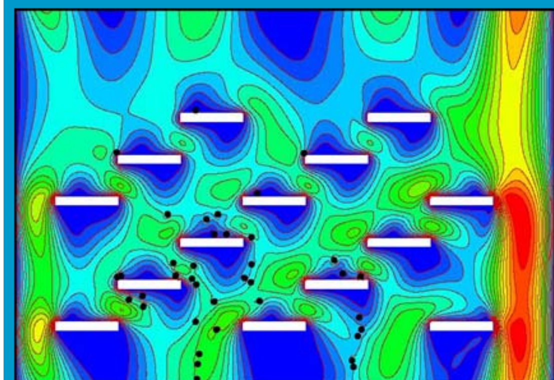

Fig 2. Particles (black dots) in a synthetic microflow device with inline obstacles. Particle attachment on inline obstacles (white rectangles) is active. Contours represent flow velocity (model result).

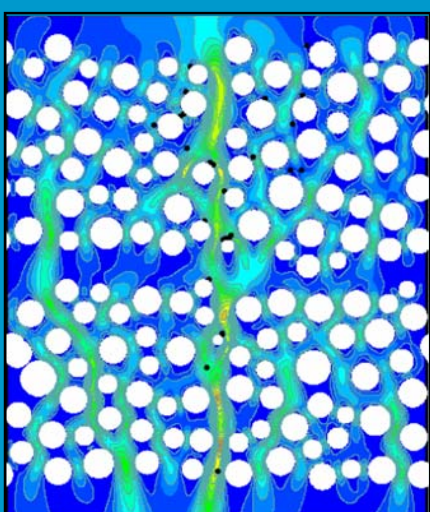

Fig. 3. Particles (small black dots) in a fractured porous medium. Particle attachment on grains (large white dots) is active. Contours represent flow velocity (model result).

Project Brief

Problem Statement: Existing continuum-based colloidal transport models use empirical effective parameters to simulate various aspects of colloidal transport processes at a phenomenological level. Such models do not adequately address the hydrodynamic processes governing particle trajectories due to channel-wall roughness, lubrication forces, and wall and inertial effects. Nor do they incorporate chemical and physical processes such as particle attachment on fracture-wall surfaces due to the Brownian effect and particle migration in geometrically complex flow paths. These processes, however, may significantly affect the retardation and migration paths of colloidal particles.

Approach and Accomplishments: We are developing computationally efficient (parallelized) 2D and 3D simulation capability to simulate trajectories of multiple inert and reactive particles and their immobilization on channel walls and inline obstacles. The simulation capability is based on the lattice-Boltzmann (LB) method. This method was chosen for its computational efficiency and ease of handling complex flow domain geometries. The simulation capability is being used to quantify the effects of particle sizes and shapes, release locations and rates, flow regimes, particle-wall interaction potentials, and particle and wall surface heterogeneities on particle trajectories in complex flow systems. We have recently incorporated new simulation features involving (i) two-body van der Waals and electrostatic forces between particles; (ii) a harmonic-spring model for particle attachments on channel walls and obstacles; (iii) an immerse boundary model for simulating softer particle-wall interaction; and (iv) a modified LB formulation to account for stochastic behavior of particles.

To test the new simulation capability, microscale laboratory experiments under different flow regimes are being conducted and the results will be compared to simulation results. To date, multiple-particle simulations in both porous and fractured media were able to capture particle behavior in slow and fast flow paths, as has been observed in our experiments and reported in the literature.

Client Benefits: Enhanced simulation capabilities will provide more reliable colloidal transport analyses supporting safety and performance assessments of potential geological repositories and optimal design and delivery of reactive agents via engineered particles to targeted sites in biomedical and subsurface biomedical applications.

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