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Modeling and Simulations of Particulate Flows through Functionalized Porous Media[1] CHUNHUI LI, PRASHANTA DUTTA, JIN LIU, Washington State University — Transport of particulate fluid through a functionalized porous material is of significant interest in many industrial applications, such as earth sciences, battery designs and water/air purifications. The entire process is complex, which involves the convection of fluid, diffusion of reactants as well as reversible chemical reactions at the fluid-solid interface In this work we present a convection-diffusion-reaction model and simulate the transport of particulate fluid through a functionalized porous media. The porous structures are generated and manipulated through the quartet structure generation set method. The Navier-Stokes with convection-diffusion equations are solved using the lattice Boltzmann method. The chemical reactions at the interface are modeled by an absorption-desorption process and treated as the boundary conditions for above governing equations. Through our simulations we study the effects of porous structures, including porosity, pore orientation, and pore size as well as the kinetic rates of surface reactions on the overall performance of removal efficiency of the species from the solution. Our results show that whole process is highly affected by both the porous structures and absorption rate. The optimal parameters can be achieved by proper design.

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