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Modeling of nanoparticle transport and deposition in a porous medium: Effects of pore surface heterogeneity[1] NGOC PHAM, The University of Oklahoma, DIMITRIOS PAPAVASSILIOU, The University of Oklahoma & NSF — Pore surface charge heterogeneity has been found to affect particle retention in flow through porous media. In this study, retention of nanoparticles under different surface blocking conditions is numerically investigated. Micro-CT scanning is used to reconstruct the 3D geometry of sandstone and image-based analysis is used to characterize the pore space and the mineral composition of the rock. Flow of water through the sample is simulated with the lattice Boltzmann method. The motion of nanoparticles is modeled by injection of particles moving under convection and molecular diffusion and recording their trajectories in time [1,2]. When interacting with the pore surface, particles can be retained onto the surface with a particular deposition rate. As deposited particles hinder the retention of other particles by blocking occupied sites, the deposition is considered to be a second order process. Particle breakthrough under different modeled and real distributions of surface heterogeneity as a function of various surface blocking conditions is investigated. The effect is stronger when parts of the surface are much more favorable for deposition than others.

[1] Voronov, R.S., VanGordon, S., Sikavitsas, V.I., Papavassiliou, D.V., *Int. J. Num. Metods in Fluids,* **67,** 501, 2011
[2] Pham, N., Swatske, D.E., Harwell, J.H., Shiau, B.-J., Papavassiliou, D.V., *Int. J. Heat & Mass Transf.*, **72,** 319, 2014

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