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Lattice Boltzmann simulation of electrostatic double layer interaction force for nanoparticles[1] GRACE X. SHI, YAN JIN, VOLHA LAZOUSKAYA, CHAO WANG, LIAN-PING WANG, University of Delaware — Modeling the transport and retention of nanoparticles (NPs) through soil porous media requires an accurate description of the electrostatic interaction force between a nanoparticle and soil grain. In this study, we apply the lattice Boltzmann method to directly solve the nonlinear Poisson Boltzmann (PB) equation for several geometric configurations including plate-plate, NP-plate, and NP-NP interactions, for any surface potentials and interaction distances and for different boundary conditions. Interaction energy and force are then derived from the simulations. For the case of plate-plate interaction, the simulation results are compared to the exact solution of the nonlinear PB equation. It is shown that the linear PB solution is valid when the nondimensional surface potential is less than one, and that the linear PB solution over-predicts the interaction force for intermediate gap distances but under-predicts the force for small gap distances. For NP-plate and NP-NP interactions, an axisymmetric lattice Boltzmann formulation is developed to solve the governing equations. The results will be compared to the classic approximate expressions of interaction force to evaluate their validity and to study the effect of nanoparticle size.

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