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Multiscale modeling of ion transport in water saturated nanostructures of clays

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Ion diffusion within clays is a fundamental process related to contaminant transport in groundwater and radionuclide migration in the context of nuclear waste disposal. Montmorillonite, one of the predominant minerals within bentonitic clays, exhibits distinguished physicochemical properties such as the ability to absorb water and ions, accompanied by underlying swelling. This behavior is primarily governed by the electrical double layer (EDL) effect at the nanoscale. In turn, these nanoscale interactions have a critical influence on the macroscopic transport properties in clays. In this study, a multiscale modeling technique was developed to combine molecular-scale and pore-scale modeling. At the molecular scale, a coarse-grained (CG) mesoscale model was used to generate the nanostructures of sodium montmorillonite, where ClayFF force-field atomistic montmorillonite platelets are equivalently represented by coarse-grained platelets including two types of particles: central nonhydrogen-bonded particles and edge hydrogen-bonding particles (1). At the pore scale, the lattice Boltzmann method (2) is used to solve the coupled Poisson-Nernst-Planck equations on GPUs to model the transport of ions in the nanostructures obtained by the CG mesoscale model. Since the variable charge of the edges of the montmorillonite platelets depends on the pH, an inhomogeneous surface charge density is employed as a boundary condition to obtain the electric potential distribution. Quantitative analyses carried out by this multiscale model were implemented to investigate the influence of clay density, ionic strength, and pH on the effective diffusivities of ions. The insights into the ion transport process and the effect of edge sites in clays gained in this study can be implemented in larger-scale analyses such as continuum-scale reactive transport simulations for radionuclide migration in deep geological repositories for radioactive wastes.

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