MOLECULAR DYNAMICS SIMULATION OF INTERACTIONS BETWEEN CLAY MINERALS AND A CONTROLLED ORGANIC PHASE

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ABSTRACT

Engineered organoclays are 2:1 phyllosilicate soils that have been synthesized with a controlled interlayer organic phase to exhibit enhanced strength, lower compressibility, and stronger retention of organic compounds. Engineered organoclays are highly sorptive, and have a variety of potential engineering applications as sorbents or amendments in engineered earthen barrier systems. Previous studies examined the impact of the organic coating on a soil’s physical properties; however, the geochemical behaviors of organoclays, especially their interaction with organic compounds at the micro-scale, remained relatively unquantified. This study investigated the engineering behavior of montmorillonite modified with a variety of quaternary ammonium cations (QAC clays) with controlled structure and density of loading. Molecular dynamics simulations were used to model the surfactant arrangement, geochemical processes in the QAC-clay interlayer, including organic compound sorption and mass transport, as well as the surface electrokinetics of suspended QAC-clay particles. All simulations were carried out based on the combined force field of ClayFF and the Consistent-Valence Force Field to ensure the accuracy of the simulation results, and results yielded insight into the prediction of synthesized QAC-clay behaviors as sorptive material for non-polar organic compounds.