

Mechanical properties of swelling clays are influenced by clay-fluid molecular interactions

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Abstract:

Swelling clays, also known as expansive clays, are found all over the world. These clays swell and exert enormous swelling pressures when they come in contact with water. These clays are also used as barrier materials in landfills and other containment systems to prevent contaminants from moving into underlying soils or groundwater. The swelling of these clays is accompanied by significant changes to their mechanical and hydraulic conductivity properties. Our previous workⁱ has shown that the swelling clay's permeability is strongly influenced by the molecular interactions between the clay and the soil pores' fluid. In the present work, we describe the role of clay fluid molecular interactions on the compressibility and shear strength of swelling clays.

Atomistic models of sodium montmorillonite clay are constructed. The models include two clay layer models and ten clay layer tactoid models. These models mimic the structures and charges of SWy-1 and SWy-2 clays used in our experimental work. Fluid molecules of fluids with a wide range of dielectric constants 110 to 2.4, representing highly polar to nonpolar fluids, were introduced in the smectite clay's interlayer. The fluid content varied from zero to 30%. Steered molecular dynamics simulations were conducted to apply a range of compressive stresses to the clay surface. We evaluated the compression of the interlayer and the conformation of the fluid molecules in the interlayer. The compressibility of the clay is reduced with the increasing dielectric constant of the fluid. Interaction energies between the fluid molecules and the various constituents of the clay were evaluated to elucidate the fundamental mechanisms that influence the swelling clays' compressibility. Additionally, we evaluated the clay interlayer's shear response with the fluids, and again the shear response of the clay was strongly influenced by the fluid polarity.

A new device to evaluate the compressibility of swelling clays with the various fluids was designed and fabricated. The experiments also indicated that the clay is more compressible with decreasing fluid polarity. Innovative nanoindentation experiments and unconfined compression strength experiments were conducted to evaluate the shear response of the clay for various magnitudes of swelling. The modeling and experiments provide an insight into the mechanisms that influence the mechanical response of the swelling clays and the critical role of clay-fluid interactions in influencing the responses.

ⁱ Amarasinghe, P. M.; Katti, K. S.; Katti, D. R., Insight into Role of Clay-Fluid Molecular Interactions on Permeability and Consolidation Behavior of Na-Montmorillonite Swelling Clay. *Journal of Geotechnical and Geoenvironmental Engineering* 2012, 138 (2), 138-146.