Properties of clay-rich fine-grained sedimentary rocks from large scale Molecular Dynamics simulations

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Fine-grained sedimentary rocks play an important role in a wide variety of modern energy technologies: from petroleum geology; geological carbon sequestration; to radioactive waste management. Yet, despite their utility and ubiquity, many of their properties remain poorly understood. In particular, the ability to predict the permeability of such fine-grained sedimentary rocks remains one of the largest fundamental challenges in the geosciences with potentially transformative implications.

In the present work, we show how large-scale classical molecular dynamics simulations can be used to help interpret the phenomenon of nanoscale diffusion within fine-grained sedimentary material. All-atom simulations containing multiple discrete clay particles are utilized to understand the roles of dry bulk density (porosity) and pore water chemistry (charge-balancing cation and pore water salt composition) on the microstructural, mechanical and transport properties of the overlying clay matrix. Special emphasis is placed on comparing our results with the available experimental data.

Microstructural properties (pore size distribution, tortuosity, anisotropy), mechanical properties (viscosity) and transport properties (diffusion coefficients of water and ions, electrical conductivity, dielectric relaxation and hydraulic permeability) are all calculated and compared to experiment. The anion exclusion between the clay particles is calculated and compared against both experimental data and several theoretical models.