

Molecular dynamics simulations of propane-water mixtures confined in cylindrical silica pores

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Despite the extensive length and time scales over which fluid-mineral interactions can occur, interfacial phenomena control the exchange of matter and impact the nature of multiphase flow and reactive transport of C-O-H fluids in geologic systems. In general, the properties of confined geofluids, and their influence on porous geologic materials are much more poorly understood than those of bulk fluids. To improve upon the state of the art, we employed equilibrium molecular dynamic simulations to study propane diffusivity inside a 16 Å diameter cylindrical pore carved out of amorphous silica. All the dangling silicon and oxygen atoms were saturated with hydroxyl groups and hydrogens which results in a total surface density of 3.8 –OH/nm². Simulations were performed at 300 K, at different bulk propane pressures, and varying the amount of water present. The distribution of the molecules within the pore was analysed from the simulated trajectories, which allowed us to quantify the hydrogen bond network and the segregation of propane near the pore center. The mean square displacement was used to quantify self-diffusion coefficients. Propane diffusivity in the cylindrical pore was found to depend on pressure, as well as on the amount of water present. In particular, we found that the propane self-diffusion coefficient decreases with increasing water loading. The results are in quantitative agreement with neutron scattering data conducted for propane-water systems confined in MCM-41 – type materials. The synergistic comparison of simulations and experiments allows us to better understand the molecular phenomena responsible for the observed results. The data are useful for better understanding the migration of fluids in the subsurface.