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Aqueous Hydrogen Sulphide in Slit-Shaped Silica Nano-Pores: Confinement Effects on Solubility, Structural and Dynamical Properties

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Abstract : It is known that confinement in nm-size pores affects many structural and transport properties of water and co-existing volatile species. Of particular interest for fluids in sub-surface systems, in catalysis, and in separations are reports that confinement can enhance the solubility of gases in water. Equilibrium molecular dynamics simulations were performed for aqueous H_2S confined in slit-shaped silica pores at 313K. The effect of pore width on the H_2S solubility in water was investigated. Other properties of interest include the molecular distribution of the various fluid molecules within the pores, the hydration structure for solvated H_2S molecules, and the dynamical properties of the confined fluids. The simulation results demonstrate that confinement reduces the H_2S solubility in water and that the solubility increases with pore size. Analysis of spatial distribution functions suggests that these results are due to perturbations on the coordination of water molecules around H_2S due to confinement. Confinement is found to dampen the dynamical properties of aqueous H_2S as well. Comparing the results obtained for aqueous H_2S to those reported elsewhere for aqueous CH_4, it can be concluded that H_2S permeates hydrated slit-shaped silica nano-pores faster than CH_4. In addition to contributing to better understanding the behavior of fluids in subsurface formations, these observations could also have important implications for developing new natural gas sweetening technologies.

Keywords : confinement, interfacial properties, molecular dynamic simulation, sub-surface formations
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