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Molecular Simulation Study of Swelling Clays

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Grand canonical Monte Carlo and molecular dynamics simulations were applied to understand the molecular mechanism of species transport in clays. The variation of clay basal spacing as a function of relative humidity predicted based on the swelling free energy profiles was consistent with X-ray data. The hydration of clays shows the following well-known order: Mg2+ > Ca2+ > Sr2+ > Li+ > Na+ > K+. The diffusion of water and ions generally increases with relative humidity in all samples. Swelling due to H2O intercalation processes could lead to permeability changes that directly impact successful storage of carbon dioxide. We observed a favorability of adsorption of CO2 (or CH4 to a lesser extent) by clays at intermediate preadsorbed water contents. At low pressures, the adsorption amount of CO2 (or CH4 to a lesser extent) in the small pore was higher than that in the larger ones. The preadsorbed water content affects competitive sorption of methane and carbon dioxide onto clays. Our molecular simulations demonstrate that CO2 has a higher affinity for clays and will therefore displace adsorbed CH4. The ideal adsorbed solution theory agreed well with the adsorption capacities and selectivities of CO2/CH4 mixture. The mobility of CO2 in the interlayers of clays, at fixed loading of CO2, is not much affected by CH4. The presence of adsorbed CO2 molecules, at fixed amount of CH4, very much reduced the self-diffusion coefficients of CH4, and relatively larger decreases in those coefficients are acquired at higher loadings. At reservoir conditions, the adsorption of CO2 in the dehydrated interlayer is inhibited, followed by the expansion of the interlayer space due to uptake of water and CO2 as the relative humidity increases. The type of cation does not affect much the mobility of CO2 in each hydration state in accordance with the fact that CO2 molecules rarely move into the first hydration sphere of the interlayer cations.

References

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