Water/Brine Films Govern Fluid Transport in Aromatic-Filled Nanopores

Anh Phan [C, S] and Alberto Striolo
Department of Chemical Engineering, University College London, London, United Kingdom
anh.phan.13@ucl.ac.uk

The interactions of trapped reservoir gases within organic-rich sedimentary rocks have direct relevance to many geo-energy applications. Among the nanoscale properties that play most significant roles in determining the efficiency of such applications are fluid adsorption capacity, oil displacement efficiency, and fluid transport. Employing molecular dynamics, we examine here adsorption and transport of gases containing CH_4 and either CO_2 or H_2S with amorphous silica nanopores filled with benzene. We explicitly quantify the effect of small amounts of water/brines at geological temperature and pressure conditions. Because of wetting, the presence of brines lessens the adsorption capacity of the aromatic-filled pore. The simulation results show salt-specific effects on the transport properties of the gases when either KCl or $CaCl_2$ brines are considered, although adsorption was not affected. The acid gases considered either facilitate or hinder CH_4 transport depending on whether they are more or less preferentially adsorbed in the pore as compared to benzene, and this effect is mediated by the presence of water/brines. Our simulations confirm that shale gas-organic matters-rock interactions can be strongly modified by the presence of brines. It is discussed how simulation results could be used to extract thermodynamic quantities that in the future will help optimise the transport of the various gases through organic-rich and brine-bearing sedimentary rocks, which is likely to have positive impact on both hydrocarbon production and carbon sequestration applications.