A Molecular Dynamics Simulation Approach in Estimating Organic-rich Shale Permeability

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Abstract

Permeability is important in quantifying flow capacity in petroleum reservoirs. Gas shale permeability is challenging because transport in organic nano-porous media has not been fully understood yet. We performed nonequilibrium molecular dynamics simulations of steady-state methane flow in single-wall carbon nanotube based on a moving piston model (Riewchotisakul and Akkutlu, 2015). The piston model allows us to observe transition from convection to molecular (pore) diffusion under the reservoir conditions and to understand the effects of adsorbed methane molecules on the overall transport in the tube. Based on molecular simulations, we show that adsorbed gas molecules by organic nano-capillary walls are mobile and this significantly enhances the overall mass flux inside the capillary. Contribution is more significant in smaller capillaries.

In the second part of the paper, we considered steady-state transport across a pore-network of inter-connected nano-capillaries. The preliminary simulation results show that the modified Hagen-Poiseuille equation leads to representative elementary volume of a model kerogen. The estimated permeability of the volume is sensitive to surface properties of the nano-capillary walls indicating that fluid-wall interactions driven by molecular forces could be significant during the large-scale transport within kerogen.