Viscosity and flow structure of hydrocarbons in slit pores

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The work studies the structure and viscosity coefficients of hydrocarbons liquid in slit pores. The molecular dynamics (MD) method is used. The model liquids are *n*-pentane and *n*-dodecane, and the walls composed of layered minerals pyrophyllite and montmorillonite are considered. The hydrocarbons are modeled using the OPLS-AA forcefield with 1.14*CM1A charge corrections [1] and the minerals with ClayFF forcefield [2].

The viscosities are calculated by enforcing Couette flow between the pores, which allows one to compute viscosity and estimate the slip length. The simulations show no significant effect of the pore width on the viscosity-density dependence of hydrocarbons, even when pore width is less than 4 nm. Pores with pyrophillite walls without water and ions on surface show the effect on structuring the hydrocarbon molecules close to surfaces. Pores with montmorillonite walls which have water and Na ions on the surface have a significantly weaker structuring effect on the confined hydrocarbons. However, the slip length of *n*-pentane is larger in the pyrophyllite pores then in the montmorillonite pores, 0.3 nm and less than 0.1 nm, respectively. The lower slip is probably due to interaction with water on the surface and the surface charge in montmorillonite.

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[2] Cygan R T, Liang J J and Kalinichev A G 2004 *J. Phys. Chem. B* **108** 1255–1266