

Transport properties of confined hydrocarbons in slit pores

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The transport properties of liquid hydrocarbons in slit pores between layers of clay minerals are studied using non-equilibrium molecular dynamics methods. Hydrocarbons and walls are simulated with the OPLS-AA-1.14*CM1A [1] and ClayFF [2] force fields, respectively, and pore widths from 2 to 7 nm are considered.

Non-equilibrium molecular dynamics simulations are performed for Couette and Poiseuille flows. For Couette flow, the Müller-Plathe approach [3] is used. To simulate a constant pressure gradient for Poiseuille flow, equal forces are applied to each molecule of the fluid. From the velocity profiles for flows, shear viscosity of the fluid and fluid-wall slip length are calculated. The viscosity-density dependencies for various pore widths are constructed by taking the Voronoi tessellation of the system and considering the total number of Voronoi cells centered on molecules of fluid as the fluid volume.

The simulations show that the viscosity-density dependence of the fluid is practically independent of the distance between pore walls, even for the smallest widths (2-3 nm). The slip length is of the order of the intermolecular distance, which can be significant for continuum simulations of fluids in nanoscale pores.

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[1] Dodda, Vilseck, Tirado-Rives & Jorgensen (2017), *J. Phys. Chem. B* 121, 3864–3870

[2] Cygan, Liang & Kalinichev (2004) *J. Phys. Chem. B* 108, 1255–1266

[3] Müller-Plathe (1999), *Phys. Rev. E* 59, 4894