Contribution ID: **891** Type: **Poster Presentation**

Structural and transport properties of hydrocarbons in clay nanopores

Thursday, 25 May 2023 15:30 (1h 30m)

Structure and transport of n-pentane and n-dodecane in clay nanopores are investigated using molecular dynamics (MD) method. OPLS-AA/CM1A force field [1] is used for hydrocarbons and ClayFF force field [2] is used to simulate pyrophyllite and montmorillonite pore walls.
The viscosity of hydrocarbons and slip lengths against the pore walls are calculated using non-equilibrium MD simulations of Couette flow. It is shown that the shear viscosity of n-pentane is only weakly affected by the pore walls for pore widths from 2 to 7 nm. The viscosity of n-dodecane increases in the pores.
The slip length of n-pentane against non-hydrated pyrophyllite walls is estimated at ~3 nm, while almost no slip is observed for n-pentane and n-dodecane against hydrated montmorillonite walls [3].
The orientational ordering of hydrocarons in pores is studied. Pentane molecules show weak ordering parallel to the walls in pyrophyllite pores and almost no ordering in montmorillonite pores with hydrated walls. On the other hand, dodecane shows strong ordering in pyrophyllite pores with molecules aligning in the same direction. The model shows a transition of n-dodecane into a state resembling liquid crystal at densities above 0.8 g/cc at 298 K [4].

The work has been supported by the Basic Research Program of the National Research University Higher School of Economics.

Participation

In-Person

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Session Classification: Poster

Track Classification: (MS13) Fluids in Nanoporous Media