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Adsorption and Transport Behaviors of Shale Oil in Kerogen Slit by Molecular Dynamics Simulation

Monday, 30 May 2022 15:10 (1h 10m)

In the last decades, shale oil, mainly distributed in organic nanopores of shale, has been considered as the representative of unconventional energy to alleviate the energy crisis. Kerogen plays a complex and key role for adsorption and transport behaviors of shale oil, and the ideal pore models greatly overestimate the flowing capability of shale oil, thus it is crucial to identify the associated mechanisms. In this paper, molecular dynamic simulation had been performed to quantify the adsorption and transport behaviors of shale oil in kerogen slits. Both the distribution of shale oil properties and potential of the mean force (PMF) were used to identify the interaction mechanisms between the light and heavy components respectively represented by methane and asphaltene. To get more accurate and reasonable flow behavior, the multicomponent shale oil in the realistic kerogen channel is studied. Both density and velocity distributions that along and perpendicular to the flow direction are studied in kerogen channel, where the influence of branch chain of kerogen is also took into consideration. We also examined the effects of different temperatures and apertures on the adsorption behavior. Owning to the extremely strong adsorption capacity between the asphaltene and kerogen, the adsorbed asphaltene layers reduce the slit width, preventing the light components from adsorbing on the kerogen slits due to the energy barrier formed by heavy components. It is found that, with an increase in temperature, the distribution of hydrocarbons performs more homogeneously. In addition, the adsorption quantity of medium components displays a reduction in kerogen slit, while the heavy component shows a rising as its greater competitive, suggesting that the medium components are the most potential fraction in thermal exploitation, and the light components keep a steady quantity with the combined action of medium and heavy components. The small slit (aperture < 2 nm) can be blocked by asphaltene molecules, and the adsorption density of hydrocarbons reaches the maximum at 2 nm aperture. On the flow direction, the velocity profile preforms the peristaltic behavior due to the effect of branch chain of kerogen, and the toluene and asphaltene components contribute it mostly. According to the heterogeneous characteristics of shale oil flow, we define the fictitious slip boundary, which corresponds to the boundary between bulk phase and adsorbed phase, to describe shale oil flow precisely. The potential energy distribution and the interaction force contour verified the peristaltic flow behavior and the validity of fictitious slip boundary.

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References

Liu J, Yang Y, Sun S, et al. Flow Behaviors of Shale Oil in Kerogen Slit by Molecular Dynamics Simulation[J]. Chemical Engineering Journal, 2022: 134682.
Yang Y, Liu J, Yao J, et al. Adsorption behaviors of shale oil in kerogen slit by molecular simulation[J]. Chemical Engineering Journal, 2020, 387: 124054.

Time Block Preference

Time Block A (09:00-12:00 CET)

Participation

In person

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