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Pore aperture regulated surface adsorption and mass transfer of hydrocarbon and CO2 in organic nanopores

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Shale oil, widely distributed in organic (i.e., kerogen) nanopores, is playing an ever-increasing role in addressing the global energy crisis, but is faced with challenges of low recovery efficiency due to well-developed nanopores. It is believed that the pore size distribution of kerogen is in the range of several angstroms to tens of nanometers (AAPG bulletin 96 (6): 1099-1119). In such a narrow pore space, oil molecules are dominated by adsorbed phase, which is hard to recover relying on pressure drop (International Journal of Coal Geology 147 (2015): 9-24). CO2 huff-and-huff is identified as a promising method to enhance oil recovery while achieving CO2 sequestration. Clarifying the adsorption and extraction behaviors of hydrocarbons in kerogen nanopores is crucial for accurately predicting oil recovery and revealing CO2 enhanced oil recovery (CO2-EOR) mechanisms.
In this work, we adopted molecular dynamics (MD) simulation to study the static spatial distribution and dynamic mass transfer of hydrocarbon and CO2 in slit-shaped kerogen nanopores by carefully designing a series of pore apertures. It shows that the adsorption and extraction behaviors of oil molecules are closely related to pore aperture. Interestingly, we found that the surface adsorption of oil molecules demonstrates a non-monotonic trend of rising after falling as the pore size decreases. Specifically, when the pore size is reduced to a certain value, oil molecules exhibit a pseudo-double layer adsorption state, in which the surface adsorption peaks of oil molecules are significantly weakened. On the other hand, although the reduction of pore width adversely affects the extraction speed of oil during CO2 soaking, the recovery efficiency presents a jump for the oil at pseudo-double layer adsorption state. Meanwhile, the surface adsorption of CO2 is also greatly enhanced, which leads to the highest CO2/Oil ratio in the nanopores. Collectively, our work provides fresh and important insights into hydrocarbon occurrence state and CO2-EOR mechanisms in organic-rich shale reservoirs and builds up a good foundation for accurate predictions of oil recovery.

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References

Characterization of gas shale pore systems by porosimetry, pycnometry, surface area, and field emission scanning electron microscopy/transmission electron microscopy image analyses: Examples from the Barnett, Woodford, Haynesville, Marcellus, and Doig units. AAPG bulletin 96 (6): 1099-1119; Oil adsorption in shale nanopores and its effect on recoverable oil-in-place. International Journal of Coal Geology 147 (2015): 9-24.

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