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Oil Displacement by Water Through an Ultra-Narrow Kerogen Pore Throat: a Molecular Dynamic Study

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Due to the continuous depletion of conventional oil reservoirs, as an unconventional reservoir, shale plays an increasingly important role to meet the ever-growing global energy demand. Thanks to the extensive number of nano-scale pores and ultra-narrow pore throats (sub-2 nm), shale media is typically subject to an ultra-low permeability. The presence of ultra-narrow pore throats in shale media can greatly reduce oil displacement by water during waterflooding. Understanding the oil displacement by water through ultra-narrow pore throats presents an enormous challenge to experimental measurements since they cannot reveal the underlying mechanism in nano-scale. On the other hand, the breakthrough pressure of oil displacement by water through pore throats has been widely described by the capillary pressure based on the Young-Laplace (Y-L) equation which is built upon a macroscopic perspective. While there have been a few molecular simulation works reported on the two-phase displacement process through inorganic pore throats with the throat widths down to 2 nm from a microscopic perspective, an explicit investigation of oil displacement by water through kerogen ultra-narrow pore throats has not been reported. In this work, we use molecular dynamics (MD) simulation to study oil (represented by octane) displacement by water through a 2-nm kerogen (represented by Type II-C kerogen) pore throat. We find that when the pressure difference between the upstream and downstream is lower than , water phase is stuck at the opening of kerogen pore throat, while the water-octane-kerogen interface curvature is dependent on . When , the water phase can displace the oil phase through the pore throat. Although the Type II-C kerogen is oil-wet based on water-oil-kerogen contact angle calculations, water has an excellent sweeping efficiency thanks to the hydrogen bonding between water and heteroatoms (such as O, N, and S) on kerogen surface. We also compared and from the Y-L equation with the contact angle and oil-water interfacial tension obtained from separate MD simulations on the water-octane-kerogen and water-octane systems, respectively. Surprisingly, from the widely used Y-L equation shows an excellent agreement with obtained from MD simulations for the 2-nm kerogen pore throat for a wide range of reservoir pressures. This work reveals underlying mechanism of oil displacement by water through an ultra-narrow kerogen pore throat from a microscopic perspective and provides important guidance to numerical modeling on oil recovery process in shale formations.

Time Block Preference

Time Block C (18:00-21:00 CET)

References

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