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Water effect on oil adsorption and configuration in nano mineral pore

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Sedimentary rock is wet in situ and generally occurs at depths in the subsurface where pores are saturated with water and hydrocarbons. The competitive adsorption of water and oil in nanopores of shales is believed to influence the dynamic configurations of fluids, and therefore their wetting and displacement behaviors and ultimately oil production. But its nature is poorly understood due to nano-confinement induced challenges in performing both physical and numerical experiments. In this study, the effects of water as a competitive adsorbate on the adsorption of n-heneicosane in Na-montmorillonite (MMT) and illite slit nanopores, with a 5-nm aperture, are systematically investigated and elucidated using molecular dynamics (MD) simulations, under realistic conditions. For each pore, water and oil molecules at selective concentrations (100%, 0), (25%, 75%), (50%, 50%), (75%, 25%) and (0%, 100%) are packed randomly into the pore at the same time and then are geometrically optimized before a stable configuration in NPT ensemble is obtained to perform MD simulation runs for estimating the density distributions for both phases.
The results show that the water molecules are the preferred adsorbate to both minerals and form an apparent wetting layer when both water and oil molecules enter the pore at the same time. These appear relatively more distinctive for the MMT than illite pores, in particular, at low water concentrations. When the oil molecules enter a pore earlier than the water molecules, or vice versa, the early-entering molecules are found to impede the late-entering ones from being absorbed onto the pore wall of MMT. The molecules, which are adsorbed to the pore wall, seem to adsorb the molecules of the other phase in the pores, to yield a smooth transition zone between adsorbed and free phases. The water molecules are found to disperse into the oil molecules, and when the water concentration is high enough, the former form bridges from one wall to another, and a film on the mineral surface. At 75% oil concentration, the oil molecules are found to be adsorbed on the wall of both MMT and illite pores but not appears as a flat film. This study offers new insight into the nature of the competitive adsorption and discusses its impact on phase configurations in pores and wetting behaviors.

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Primary author: Dr JIANG, Hang (Oil and gas resource Strategy Research Center, Ministry of Natural Resources)

Co-author: MA, Jingsheng (Heriot-Watt University)

Presenter: Dr JIANG, Hang (Oil and gas resource Strategy Research Center, Ministry of Natural Resources)

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