

Temperature, Salinity, and Oil-Water Competition Govern Shale Wettability at the Molecular Scale

Peixing Xu, Feng Yang*, Nong Kang, Sijia Nie, Jibin Fu

Hubei Key Laboratory of Oil and Gas Exploration and Development Theory and Technology, China University of Geosciences (Wuhan), Wuhan, China

Email address:

peixingxu@cug.edu.cn (Peixing Xu), fengyang@cug.edu.cn (Feng Yang), kangnongchina@163.com (Nong Kang), sijiaNie@cug.edu.cn (Sijia Nie), jibinf@163.com (Jibin Fu)

*Corresponding author

Abstract

Shale wettability is a critical interfacial property governing hydrocarbon distribution, multiphase transport, and fracturing-fluid flowback in unconventional energy reservoirs, yet its molecular response to temperature, brine salinity, and oil-water coexistence remains insufficiently resolved. This study elucidates the wetting mechanisms of representative organic and inorganic shale components using molecular dynamics simulations. Type II-C kerogen, hydroxylated alpha-quartz, and sodium montmorillonite surfaces were combined with SPC/E water, NaCl solution, and n-octane. Contact angles, molecular density and orientation profiles, hydrogen bonding, mean-square displacement, and fluid-solid interaction energies were evaluated over 278-353 K and in saline and oil-water-mineral systems. At 298 K, pure-water contact angles on kerogen, quartz, and montmorillonite were 86.73°, 25.45°, and 20.35°, respectively, establishing the hydrophilicity order montmorillonite > quartz > kerogen. Raising the temperature from 278 to 353 K strengthened water-mineral attraction and reduced contact angles by 12.55°-16.35°. In contrast, NaCl-induced hydration weakened mineral-water interactions and increased the angles to 98.54°, 56.21°, and 48.79°, with quartz and montmorillonite exhibiting greater salinity sensitivity than kerogen. The addition of n-octane further increased the three-phase water contact angles to 109.74°, 48.79°, and 39.80°. Interaction-energy analysis revealed competitive adsorption: kerogen preferentially interacted with oil, whereas quartz and especially montmorillonite retained stronger affinity for water. Oil restricted water spreading and increased water-water hydrogen bonding, while water orientation near mineral surfaces changed only slightly. These findings reveal the molecular origin of mixed wettability and provide a mechanistic basis for fluid management and hydrocarbon recovery from shale energy resources.

Keywords

Shale Wettability, Molecular Dynamics Simulation, Hydrocarbon Recovery, Kerogen, Quartz, Montmorillonite, Salinity, Oil-water Interaction