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Molecular dynamics study of the occurrence states of gas-water mixtures near the organic solid in shale reservoirs

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Abstract
Understanding the gas occurrence states under real reservoir conditions is the prerequisite to study the mechanisms of gas flow in shale reservoirs, in which large amounts of nanoscale organic pores exist. Besides, water is inevitable when considering the gas flow in shales. Thus molecular dynamics simulations were performed to study the occurrence states of gas-water mixtures near the organic solid. Results indicate that methane will approach the organic surface spontaneously, accumulate at the solid-liquid interface and form a dense gas region finally. This process has little relationship with gas saturation. Potential of mean force (PMF) was calculated to explain the enrichment of methane. We found that both the wall-gas interaction and the water-gas interaction are beneficial to the adsorption of methane and the former takes the leading role, while the gas-gas interaction impedes the adsorption. In addition, the effects of reservoir temperature, pressure, rock wettability, and carbon dioxide (CO2) on the occurrence states of methane-water mixtures near the solid surface were studied. The temperature, rock wettability and CO2 influence the occurrence states near the surface obviously, while the pressure in the simulating range does not. This study also suggests the potential of thermal exploitation, altering the rock wettability and CO2 injection to enhance shale gas recovery.
Key words shale; gas-water mixtures; organic matter; occurrence state; adsorption; potential of mean force

References

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