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Molecular dynamics investigation of water-gas two phase flow in rough clay nanopores

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The gas-liquid two-phase flow in rough nanopores plays a crucial role in shale gas extraction. To deeply understand the flow mechanisms, molecular dynamics simulation (MDS) method is often employed to simulate fluid flow in nanoscale channels. However, current researches on two-phase flow at the nanoscale have mainly focused on smooth channels. In addition, accurate simulation of the rock wall material is challenging. This work aims to investigate the mechanisms of gas-liquid two-phase flow in rough shale nanopores by using MDS.

A new rough surface model is constructed by illite crystals, and the water-gas two-phase flow is simulated in it which can achieve a more accurate characterization of flow phenomena in microscale shale reservoirs. To better represent the actual formation conditions, rough nanopores are constructed by adding roughness elements to smooth wall surfaces. Methane and water molecules are introduced into the pore models. The flow process is simulated using the EF-NEMD method. Based on these, the effects of rough particles, different arrangements of rough particles, and varying relative roughness on two-phase flow are investigated. The simulation results reveal that rough particles have a significant impact on gas-water two-phase flow. Statistical analysis is used to quantify the density, velocity distributions and boundary conditions in two-phase flow.

Simulations performed under different roughness conditions demonstrate: the presence of rough particles leads to three adsorption layers of water molecules near the pore walls; it also induces a phenomenon similar to macroscopic Jamin effect during two-phase flow, which severely affecting the flow velocity. Another important observation is that compared to smooth channels, the presence of rough particles significantly increases the boundary slip length i.e. the thickness of the immobile water layer. The different arrangements of rough particles will generate different negative slip lengths. Furthermore, with the roughness decrease the influence of rough channels on gas phase flow is negligible in hydrophilic channels. The aforementioned findings provide valuable insights into the gas-liquid two-phase flow behavior in rough nanopores, which is crucial for understanding and optimizing the transport and mass transfer processes in nanoscale systems.

This work simulates water-gas two-phase flow in rough nanopores constructed by illite crystals, which has not been previously explored. The major contribution of this work lies in analysing the impact of roughness elements on two-phase flow through MDS. It provides a basis for the development of subsequent mathematical models. Simulating the actual shale reservoir can guide the optimization of production measures. These findings provide insights into the intricate dynamics of gas-liquid two-phase flow in rough channels and contribute to a better understanding of fluid transport in porous media with real-world applications, such as shale reservoirs.

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References

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