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Investigation of Fluid Flow Mechanism Considering Multi-Component Fluids, Nanopore Roughness, and Nanopore Flexibility

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Understanding the occurrence and flow mechanisms of shale oil in nanopores, as well as the impact mechanisms of fluids on solid deformation, is crucial for advancing our comprehension of fluid behavior in porous media. Prior neglect of factors such as the multi-component characteristics of shale oil, the properties of real shale nanopore walls, and nanopore flexibility has resulted in insufficient knowledge regarding the occurrence and flow mechanisms of shale oil in nanopores. In this study, molecular dynamics simulations were employed to extensively investigate the occurrence and flow mechanisms of fluids in graphene, hydroxylated quartz, rough kerogen rigid nanoslits, and flexible nanotubes. The following conclusions were drawn: (1) The occurrence patterns of multicomponent shale oil in organic and inorganic nanopores were revealed. The adsorption characteristics of shale oil are related to the pore wall elements. Components containing oxygen, nitrogen, and aromatic hydrocarbons tend to adsorb more readily on quartz surfaces, while sulfur-containing components also tend to adsorb on the kerogen surface due to interactions with sulfur elements in kerogen. (2) Real shale oil flows in real nanopores without slippage. Through simulations comparing the flow of single/multicomponent shale oil in smooth/rough nanopores, we found that slip phenomena occur only under ideal conditions (single-component oil, smooth surface). The slip does not occur in realistic shale oil flow, offering theoretical support for setting slip length in pore-scale simulations. (3) In quartz, kerogen, and graphene nanoslits, an increase in pore pressure was observed with the elevation of pressure gradients. In rigid graphene nanoslit, fluid flow induces an elevation in nanoslit pressure, with a critical pressure gradient of 1 MPa/nm. Below this threshold, pore pressure exhibits minimal variation; above it, a significant increase is observed. Higher pressure gradients lead to an increase in kinetic energy in the direction perpendicular to the wall, indicating an escalation in collision intensity between the fluid and the wall, as well as among fluid particles, resulting in a rise in pore pressure. Increased pressure gradients reduce the interaction energy between the fluid and the wall, signifying that fluid molecules are propelled further from the wall upon collision, underscoring the gradual intensification of fluid-wall collisions. (4) The intricate relationship between pressure gradient, nanopore stress, and nanopore strain was revealed. Under static conditions, the transition of a rigid and smooth nanopore to a flexible one can result in an increase in surface roughness, which leads to a reduction in the density of the adsorption layer. The pore width decreases and the pore pressure increased slightly. Fluid flow induces an increase in pore pressure and width. Simulations of fluid flow in rigid nanoslits with coupled pore width and rock compressibility, as well as in flexible nanotubes, indicate that an increase in pressure gradient leads to pore expansion. This study revealed the intricate interactions of shale oil in nanopores, offering theoretical support for understanding its flow in porous media and contributing to the efficient extraction of shale oil from unconventional reservoirs.

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