Pressure-dependent transport characteristic of methane gas in slit nanopores

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Abstract

Because of the large amounts of reserves and wide distribution, shale gas draws more and more attentions and significantly influences the pattern of the global energy industry in past decades, leading to the worldwide “shale revolution”. However, the transport mechanism of methane gas through the nanopores is still unclear. Shale gas is mainly stored in nanopores of shale formations over a wide range of pressure which is a fundamental thermodynamic variable dominating the properties of substances, rendering that it is important to understand the pressure-dependent transport characteristic of gas molecules in nanopores. Toward this end, we performed molecular dynamics (MD) simulations to investigate the transport characteristic and its mechanism of methane gas in slit nanopores under different pressures. A modified bin method considering local gas density was proposed to reveal the mass velocity profile of methane gas in nanopores. Combining the trajectories of representative molecules, we found that the underlying mechanism of methane gas transport characteristic behaves as the competition between gas intermolecular collisions and gas-wall interactions. The transport characteristic of methane gas in slit nanopores is dependent on the pressure. Meanwhile, the pore width can significantly influence the mass flux contributions of different transport mechanisms. Under the high pressure, viscous flow is the primary transport mechanism due to the frequent gas intermolecular collisions. Under lower pressure and in larger nanopores, Knudsen diffusion becomes the dominating transport mechanism due to the enhancement of gas-wall interactions (collisions). Narrower nanopores can significantly increase the mass flux contribution of surface diffusion due to the increased proportion of absorbed gas molecules. In particular, we proposed a theoretical model coupling multiple transport mechanisms, which can accurately predict the apparent permeability of methane gas in slit nanopores. Under lower pressure and in narrower nanopores, the enhancement of surface diffusion and Knudsen diffusion can increase the apparent permeability of methane gas by as much as 50 times or more, demonstrating the sensitivity of pressure and pore size for methane gas transport.

Keywords: **Shale gas; Pressure; Transport characteristic; Transport mechanism; Molecular dynamics simulation**