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Determination of the type of free gas transport in shale gas formations based on Knudsen number from molecular perspectives

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The type of free gas transport in shale gas formations includes viscous flow, slip flow, and Knudsen diffusion. These three types of transport are categorized based on Knudsen number (Kn), which is defined as the ratio between the mean free path (MFP) of gas and the pore width. The MFP of gas in nanopores is usually estimated based on the ideal gas model. However, the gas in the nanopores is not evenly distributed due to the interactions between gas and walls, and thus the gas in nanopores cannot be viewed as ideal gas, meaning the real value of Kn may deviate from the value obtained by ideal gas model. In this study, we calculated the Kn of methane (CH4) in nanopores by molecular dynamics simulations. The values of MFP in nanopores were obtained based on the trajectories of CH4. We investigated the proportions of viscous collision, slip collision and Knudsen collision, which determine the type of gas transport. By analyzing the proportions of forementioned three types of collision for different values of Kn in nanopores, a real criterion for determining the type of free gas transport was established. Results show that, at 353.15 K with the pressure lower than 50 MPa, the value of Kn of CH4 is smaller than 0.1 in the pore with the width less than 5 nm. The major type of CH4 flow is the viscous flow when Kn < 0.07, and the slip flow should be considered when Kn > 0.07. The Knudsen diffusion cannot be ignored when Kn > 0.08. The results obtained in this study are crucial for correctly determining the type of gas transport in shale formations.

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Primary authors: Mr ZHAO, Xinyi (China University of Petroleum (East China)); Ms SANG, Qian (China University of Petroleum (East China)); Mr SUN, Hai (China University of Petroleum (East China)); Mr YAO, Jun (China University of Petroleum (East China)); Mr DONG, Mingzhe (China University of Petroleum (East China))

Presenter: Mr ZHAO, Xinyi (China University of Petroleum (East China))

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