Molecular Dynamics Simulation of Slip Flow in Nanopores for Shale Gas Development

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Slip phenomenon is one of major characteristic of gas flow through narrow pore throat, such as tight sands, coal seams, and shale formations. Consequently, permeability correction need to be considered for evaluating the flow ability of gas in these reservoirs. There are various analytically derived correction models for engineering applications. However, it is not well understood which one should be applied to real shale reservoirs.

Slip velocity and permeability correction for gas flow in nanopores are studied by molecular dynamics simulations (MD). For simplicity, the considered system is methane gas flow in parallel plate channel of quartz and pyrophyllite. The fluid flow is characterized by the Knudsen number. The simulation results show that the relations between slip velocity (normalized by the maximum velocity) versus Knudsen number and between permeability correction factors versus Knudsen number agree well with Beskok and Karniadakis' analytical solution (BK model) for large nanopores (10-34 nm) . However, some deviations from BK model were noted for small nanopores (2-10 nm), where the deviation from BK model became significant. We suggest that the limit for application of BK model may be about 10 nm, and it is ascribed to the fact that the overall fluid is no more homogenous (the fluid is structured in the proximity of the walls due to the interaction from the wall molecule). Although these trends are same in both of quartz and pyrophylite channel, the slip velocity in quartz channel is slightly smaller than that in pyrophyllite channel for small nanopores (< 10 nm). It is considered that the slip velocity decreases as the roughness height becomes large compared to the mean free path, especially in quartz channel which has atomistically more rough surface.

MD simulation results confirmed that direct application of BK model is very good down to about 10 nm and further suggested a correction for small nanopores (< 10 nm). These findings could be extended to multiscale simulations with the reconstructed porous structures of shales by FIB-SEM imaging.