Research highlight

Investigation of shale gas flows under confinement using a self-consistent multiscale approach

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Abstract:
This report summarises our recent findings on non-ideal gas flow characteristics in shale nanopores facilitated by our strongly-inhomogeneous kinetic model. As there are a significant portion of nano-scale pores in shale, gas molecule size is comparable to both the gas mean free path and the characteristic length of the flow domain, and various factors including fluid-solid and fluid-fluid interactions, pore confinement, surface roughness, and non-equilibrium effect need to be considered in a self-consistent manner. These factors are either considered in the governing equation according to the dense gas and mean-field theories, or through the boundary condition based on molecular dynamics simulations. Our kinetic model results are consistent with the molecular dynamics data at the molecular scale and converge to the continuum predictions when pores become large. This model serves as an accurate tool to investigate multiscale transport of shale gas and is helpful for upscaling from the microscopic to continuum levels with a firm theoretical basis.

For practical shale gas flow simulations, a plethora of nanoscale effects need to be considered. The most common one is the rarefaction effect, which is characterised by the Knudsen number (Kn). In the continuum flow regime, gas flows can be described by the continuum theory, while a slip boundary condition (BC) is additionally needed in the slip flow regime. In the more rarefied regimes, the continuum assumption becomes invalid and the Boltzmann equation (BE) is solved to describe the flow. However, the BE is based on the assumption that gas molecule size is negligible comparing to gas mean free path (MFP), which is not true for shale gas flows in nanopores (Wu et al., 2016, Shan et al., 2021).

As gas molecule size is comparable to both gas MFP and pore sizes in shale (as shown in Fig. 1(a)), the Enskog theory for dense gases is more appropriate to capture the non-equilibrium effects (Wu et al., 2016), where the volume exclusion is considered. Volume exclusion changes the collision frequency between molecules through reducing the free space

for molecular motion and the shielding effect. As pointed out by Luo (1998), this volume exclusion needs to be considered explicitly for non-ideal gas flows, rather than merely changing the relaxation time. However, the intermolecular attraction is not considered in the original kinetic theory for dense gases. The mean-field theory considers a particle to move under an effective force potential due to intermolecular attraction (He and Doolen, 2002). Therefore, combining dense gas theory and mean-field approximation, a self-consistent approach can be established to describe non-ideal gas flows. In this framework, the fluid-fluid molecular interactions are the microscopic description of real gas effect at high pressure, which is often considered by the real gas equation of state at the macroscopic level.

Gas adsorption arising from fluid-solid interactions is another key mechanism for gas transport in shales. On one hand, gas adsorption is an important storage form in shale reservoirs, which can significantly increase the amount of stored gas. On
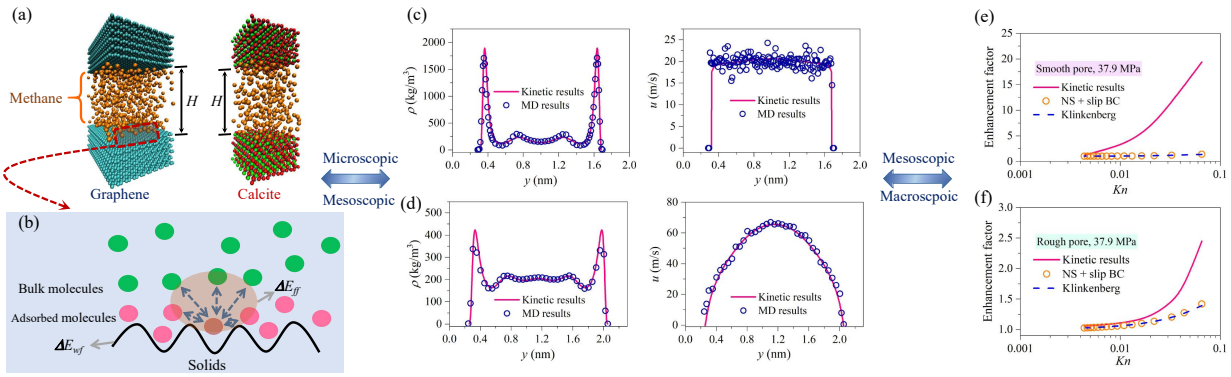
Fig. 1. Kinetic model bridges the molecular dynamics (MD)and continuum results (adapted from Shan et al., 2011, 2022): (a) gas flow in smooth and rough nanopores; (b) continuum description of solid/fluid interactions; (c) and (d) kinetic and MD results in smooth and rough pores; (e) kinetic and continuum results in nanopores.

the other hand, the existence of gas adsorption may change gas transport characteristics due to its distinct difference from free gases. Furthermore, gas adsorption is affected by pressure, temperature, wettability etc., which play different roles during the whole lifetime of gas production. A fluid-solid interaction potential is included in the strongly inhomogeneous kinetic model (Guo et al., 2005) to describe the physical adsorption process, which is proved to be consistent with MD, but in higher computational efficiency (Shan et al., 2021).

Another challenge in modelling of nanoscale fluid flows is the lack of an appropriate BC to accurately capture molecular-scale slip behaviours. At the nanoscale, the BC should specify the interactions between fluid-solid molecules and bulk-adsorption molecules, as shown in Fig. 1(b). Recently, a molecular-kinetic BC was proposed to solve this problem (Shan et al., 2022). The slip occurs at the interface between the adsorbed gas and solid surface, which is commonly called surface diffusion. Together with appropriate governing equations, the non-ideal gas dynamics from nanoscale to continuum scale can be modelled accurately.

The kinetic model has been solved numerically via the discrete unified gas kinetic scheme (Shan et al., 2020). According to our study, the kinetic results agree well with the MD data for gas flows at the nanoscale confined by both smooth and molecular-scale rough surfaces, as shown in Figs. 1(c) and 1(d), respectively. Gas adsorption forms close to the wall, where a significant slip velocity exists when wall surfaces are smooth. By contrast, slip velocity at the surface becomes smaller or even disappears in rough nanopores. While our kinetic model can capture nanoscale gas dynamics as accurately as MD, it can also describe gas flow behaviours in the continuum limit. As shown in Fig. 1(e) and 1(f), our kinetic results converge to the results of the continuum theory, as *Kn* decreases and the nano-confinement effects become less important.

Overall, gas flow behaviours can be accurately described by our kinetic model with a molecular-scale slip BC by consistently considering the real gas, confinement and non-equilibrium effects, which provides a promising multiscale approach to studying flow physics from nanoscale to macroscale, circumventing the restrictions of MD at the molecular scale and the continuum theory at the continuum scale.

Acknowledgements

Conflict of interest

The authors declare no competing interest.

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