Pore-scale simulation of methane transport in complex nanopores using a stabilized lattice Boltzmann method

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Abstract

The efficient development of shale gas reservoirs requires an accurate understanding of methane gas transport in the matrix whose pore size is mainly in the nanoscale range. As a result, continuum-based approaches may be inadequate in simulating flow in such systems. Molecular dynamics (MD) simulations are capable of capturing the relevant microscale physics with high fidelity, albeit at a substantial computational cost. This high expense restricts MD simulations to rather small systems and computational domains, which may not be representative of complex hierarchical nature of shale reservoirs. To bridge this gap, we use a particle-based approach, the lattice Boltzmann method (LBM), as a suitable means to capture the physics of transport at microscale and simulate large complex domains. In this work, the multiple-relaxation-time (MRT)-LBM is used to study methane transport in nano-size pores. The adsorption effect and non-ideal gas behavior are incorporated using the pseudopotential model and appropriate force terms. The optimal values of the LB free parameters are determined for a nano-slit pore using reference velocity and density profiles from MD simulations. A preconditioning scheme is proposed to improve the stability of LBM in the presence of force terms. In this scheme, steady-state profiles obtained in the absence of regularization are used as the initial condition for simulation runs that include the regularization step. The results show how roughness adversely affects gas-transport in nanopores. The stability of the proposed framework makes it a potential approach for studying methane transport in more complex nano-porous media and translating transport behavior across scales.

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Abstract

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