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Bridging adsorption behavior of CH4-CO2 binary systems across scales

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Adsorption of CO2-CH4 binary mixtures in permeable media plays an important role in CO2-enhanced shale gas recovery and geological storage of CO2. Grand Canonical Monte Carlo (GCMC) simulations enable the examination of the physics of adsorption in nanopores with high fidelity. GCMC tracks the motion of every molecule, which results in computational expense that rises rapidly with domain size. This limits the size of computational domains that may reasonably be simulated using GCMC. The lattice Boltzmann (LB) method is, on the other hand, a mesoscopic simulation paradigm, which tracks the statistics, i.e., distribution function, of packets of molecules instead of individual ones. As such, LB may be used to bridge scales between micro-scale (atomistic simulations) and macro-scale. In this work, we use a cubic equation of state (EoS), namely the Peng-Robinson EoS, to inform the intermolecular forces in the LB framework via a pseudopotential model. This is done in a multicomponent multiple-relaxation-time LB framework where the tunable parameters are adjusted based on benchmark atomistic simulation data. We use the validated LB model to study competitive adsorption of CO2-CH4 binary mixtures in slit nanopores. These simulations incorporate intermolecular forces and the adsorption behavior under confinement and progressively examine larger and more complex media to examine the amount of CH4 that is produced while CO2 is being stored in the media at fixed pressure and temperature conditions. The results show the dynamics of adsorption in different stages of CO2-enhanced shale gas recovery and geological storage of CO2. This multiscale simulation framework helps bridge the adsorption behavior of binary systems across scales.

Participation

In-Person

References

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