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Direct numerical simulation of CH4 - CO2 mixture flow in nanoporous media

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CO2 injection into shale is believed beneficial for both enhanced gas recovery and CO2 storage. The confined space and strong solid-molecule interactions in nanoporous media lead to different occurrence states of CH4 and CO2, causing the flow of CH4 - CO2 mixture in shale to deviate from predictions of continuum models. In this study, we employed a modified pseudo-potential based lattice Boltzmann (LB) model to study gas mixtures in nanoporous media. The mixed equation of state is used to calculate interaction force between gas mixtures. The solid-molecule interaction force is determined by comparing density profiles from LB simulation and molecular dynamics. The proposed method can model the flow of CH4-CO2 mixture in complex topological nanopores with various surface properties. Our results demonstrate that the Langmuir model and BET theory cannot accurately describe the adsorption isotherms of CH4 and CO2 in nanoporous media. The transport capacity of CH4-CO2 mixture in nanoporous media is found affected by surface properties. In organic nanoporous media, CO2 molecules tend to accumulate near the pore surface, hindering their flow compared to CH4 molecules. In contrast, inorganic nanoporous media facilitate the flow of both CH4 and CO2 molecules. We propose a modified apparent permeability model to describe the flow capacity of a CH4-CO2 mixture in nanoporous media.

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