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Lattice Boltzmann simulation of water distribution and its effect on methane adsorption in nanoporous shale

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Water vapor sorption in nanoporous media with complex pore structures, such as shale, remains poorly understood. Moreover, the initial water saturation in shale gas reservoirs affects methane's adsorption capacity, posing a challenge for accurate gas reserve estimation. Current methods, including molecular dynamic simulation, sorption experiments, and analytical modeling, have limitations in intuitiveness, research scale, and idealism, respectively.
To tackle this issue, a pseudopotential lattice Boltzmann method (LBM) is developed to explore water sorption and its impact on methane adsorption. This LBM model integrates long-range molecular forces using a modified Shan-Chen model based on the Carnahan-Starling equation of state. Validation of the LBM's simulation for water vapor sorption includes assessments of liquid/vapor densities in phase separation, vapor pressure around liquid droplets, and film thickness in parallel nanoslits using disjoining-pressure theory. For methane sorption, the LBM's validation involves lattice density functional theory and methane sorption experiments.
The findings reveal that water films in nanopores create a liquid pressure disparity of up to 100 MPa between confined and free states. Traditional adsorption theories based on simplistic pore shapes do not apply to nanoporous systems with complex geometries. In inorganic matter, hydrophilic attraction forces result in "small pores filled with liquid water and large pores covered by water film," whereas organic matter shows no water presence due to hydrophobic repulsion forces. Different water saturation levels significantly affect the relationship between pore-throat configuration and organic pore distribution, impacting effective flow pathways. The initial water saturation in shale gas reservoirs restricts methane adsorption solely to organic pore surfaces, substantially reducing available methane adsorption sites. Particularly in continental/transitional shale gas reservoirs with high clay contents, the influence of water distribution on methane adsorption needs consideration.
The proposed LBM demonstrates its ability to model sorption processes within complex porous structures efficiently. This work offers critical insights into water sorption behavior in shale's nanopore systems, laying the groundwork for modeling liquid-vapor distribution in nanoporous media at the pore scale. In addition, these findings provide theoretical support for estimating gas adsorption content and reservoir numerical simulation for shale gas reservoirs.

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References

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