



Contribution ID: 140

Type: Oral Presentation

Pore-scale prediction of CH₄-CO₂ competitive adsorption in nanoporous media coupling molecular simulation and machine learning acceleration

Thursday, 16 May 2024 14:35 (15 minutes)

In shale nanoscale pores, the CH₄ molecular size is equivalent to the mineral molecular size, then, the non-negligible gas-solid molecular interactions lead to the existence of a large amount of adsorbed gas with low mobility, which has an important impact on shale gas production. Since the adsorption capacity of CO₂ is higher than that of CH₄, the injected CO₂ can be adsorbed on the mineral surface and replace the adsorbed CH₄, becoming an effective means to increase shale gas production and a potential way to realize CO₂ geological sequestration. However, the current explanation of CH₄-CO₂ competitive adsorption is mainly limited to molecular simulation based on a single nanopore, the pore-scale competitive adsorption behavior in porous media with complex pore structure is still poorly understood and consumes a lot of computing resources.

In this paper, a multi-component lattice Boltzmann method coupled with molecular simulation and machine learning is proposed to accurately simulate and rapidly predict the competitive adsorption behavior of CH₄-CO₂ in shale kerogen and illite three-dimensional nanoporous media. Firstly, the density distribution of the miscible CH₄-CO₂ in kerogen and illite pores with different CO₂ molar fractions is calculated by molecular simulation. Then, by fitting the molecular simulated density distribution, the CH₄-solid and CO₂-solid interaction force parameters in the multi-component lattice Boltzmann model are modified, and the CH₄-CO₂ competitive adsorption in kerogen and illite porous media is simulated based on the fitting parameters. Finally, the porous media are divided into 2095 pore structures by watershed segmentation algorithm, then, the artificial neural network is trained by pore-structure characteristics and competitive adsorption capacity to accurately predict the CH₄-CO₂ competitive adsorption content in arbitrary pore structure and porous media.

This method overcomes the limitation of computing resource consumption of molecular and pore-scale simulations, and provides an effective method for the accurate simulation and rapid prediction of multi-phase multi-component competitive adsorption behaviors in nanoscale space.

Keywords: CH₄-CO₂ competitive adsorption; three-dimensional nanoporous media; lattice Boltzmann method; molecular simulation; machine learning

Indico rendering error

Could not include image: [403] Error fetching image

Acceptance of the Terms & Conditions

[Click here to agree](#)

Student Awards

Country

China

Porous Media & Biology Focused Abstracts**References****Conference Proceedings**

I am not interested in having my paper published in the proceedings

Primary author: WANG, Han

Co-author: Prof. CAI, Jianchao

Presenter: WANG, Han

Session Classification: MS09

Track Classification: (MS09) Pore-scale modelling