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