



Contribution ID: 577

Type: Poster Presentation

The Competitive Adsorption Behavior of CH₄/CO₂/H₂S Mixtures in Kerogen Nanopores from the Perspective of Molecular Simulation

Tuesday, 14 May 2024 16:05 (1h 30m)

Objectives/Scope:

Nowadays, the escalating greenhouse effect is primarily attributed to the excessive emissions of CO₂. Geologic sequestration of CO₂ and the utilization of CO₂ in displacing shale gas during gas production process could be benefit for mitigating CO₂ levels. The presence of H₂S gas in CO₂ waste emissions often poses a challenge due to the potential cost escalation associated with its purification. In response to this, the concept of CO₂/H₂S co-sequestration has been proposed, with successful implementation cases reported. However, the application of CO₂/H₂S displacement in shale gas extraction has yet to be verified. In this work, we used the Grand Canonical Monte Carlo (GCMC) method to simulate the adsorption of different components (CH₄, CO₂, H₂S in single-phase, CH₄:H₂S=1:1 in two phases, and CH₄:CO₂:H₂S=5:4:1 in three phases) within kerogen at 373.15K under various pressures. The study investigated the adsorption density, adsorption capacity, and competitive selectivity adsorption coefficients of different components on the kerogen surface. Our works could reveal the adsorption patterns of CH₄/CO₂/H₂S in kerogen pores, providing a theoretical foundation for the injection and extraction of shale gas with CO₂/H₂S.

Methods/Procedures/Process:

Adsorption behavior in ~5nm kerogen nanopores with different components systems is investigated at 373.15K and a series of pressures. The CVFF, TraPPE-EH, TraPPE-UA, and three-point potential models are used to describe the kerogen nanopores, CO₂, CH₄, and H₂S, respectively. All the GCMC simulations are completed by the MCCCSTowhee software. In the μ VT ensemble, 5000000 steps per fluid molecule are carried out to achieve equilibrium, and 10000000 steps per fluid molecule are conducted for sampling. Based on statistical data, we calculated the accessible volume, adsorption density, adsorption capacity, and competitive selectivity adsorption coefficients.

Results/Observations/Conclusions:

It was observed that CO₂ effectively reduces the adsorption of CH₄, but the introduction of H₂S significantly decreases the adsorption density of CO₂, while the adsorption density of CH₄ remains essentially unchanged. The isothermal adsorption curves reveal that the injection of both CO₂ and CO₂/H₂S leads to a reduction of approximately 50% in the adsorption quantity of CH₄, indicating effective shale gas extraction. In systems with the addition of H₂S, the adsorption quantity of CO₂ decreases by around 30% compared to systems with only CO₂ injection. The competitive adsorption coefficients of CH₄ relative to other components in different systems are all less than 1 and range between 0.2 and 0.4, suggesting a strong adsorption capacity of kerogen for both CO₂ and CO₂/H₂S.

Applications/Significance/Novelty:

This work reveals the adsorption patterns of CH₄/CO₂/H₂S in kerogen pores from a molecular perspective and provides crucial insights into the competitive adsorption patterns of CH₄, H₂S, and CO₂, which is helpful to lay a theoretical foundation for the simultaneous injection and extraction of shale gas with CO₂/H₂S.

Acceptance of the Terms & Conditions

[Click here to agree](#)

Student Awards

I would like to submit this presentation into the InterPore Journal Student Paper Award.

Country

China

Porous Media & Biology Focused Abstracts

References

[1] Zhang M, Liu Z, Pan B, et al. Molecular simulation on CO₂/H₂S co-adsorption in organic and inorganic shale nanopores. *Applied Surface Science*, 2023, 624: 157167. [2] Wu T, Zhao H, Tesson S, et al. Absolute adsorption of light hydrocarbons and carbon dioxide in shale rock and isolated kerogen. *Fuel*, 2019, 235: 855-867. [3] Chen G, Lu S, Zhang J, et al. Keys to linking GCMC simulations and shale gas adsorption experiments[J]. *Fuel*, 2017, 199: 14-21. [4] Zhang M, Zhan S, Jin Z. Recovery mechanisms of hydrocarbon mixtures in organic and inorganic nanopores during pressure drawdown and CO₂ injection from molecular perspectives. *Chemical Engineering Journal*, 2020, 382: 122808. [5] Cheng X, Cheng Y, Wang C, et al. Calculation methods on methane adsorption phase density in coal: A critical review and new insights. *Chemical Engineering Journal*, 2023: 144778. [6] Li Q, Li X, Wei N, et al. Possibilities and potentials of geological co-storage CO₂ and SO₂ in China[J]. *Energy Procedia*, 2011, 4: 6015-6020. [7] Zheng L, Spycher N, Birkholzer J, et al. On modeling the potential impacts of CO₂ sequestration on shallow groundwater: Transport of organics and co-injected H₂S by supercritical CO₂ to shallow aquifers. *International Journal of Greenhouse Gas Control*, 2013, 14: 113-127. [8] Raza A, Mahmoud M, Alafnan S, et al. H₂, CO₂, and CH₄ Adsorption Potential of Kerogen as a Function of Pressure, Temperature, and Maturity. *International Journal of Molecular Sciences*, 2022, 23(21): 12767. [9] Mudoi M P, Prusty B K. Controlling parameters of CH₄ and CO₂ adsorption on shale—a review. *Arabian Journal of Geosciences*, 2022, 15(6): 526. [10] Zhang M, Jin Z. Molecular simulation on CO₂ adsorption in partially water-saturated kaolinite nanopores in relation to carbon geological sequestration. *Chemical Engineering Journal*, 2022, 450: 138002.

Conference Proceedings

I am interested in having my paper published in the proceedings.

Primary author: BAO, Junyao (Chengdu University of Technology)

Co-authors: NING, Shaofeng (Chengdu University of Technology); CUI, Jingkai (Chengdu University of Technology); ZHAN, Shiyuan (Chengdu University of Technology); WANG, Xiaoguang (Chengdu University of Technology)

Presenter: BAO, Junyao (Chengdu University of Technology)

Session Classification: Poster

Track Classification: (MS13) Fluids in Nanoporous Media