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

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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 MCCCS Towhee software. In the μVT 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.

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