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Type: Oral Presentation

Effect of pH on the Competitive Adsorption Behavior of CO₂/CH₄ in Shale Inorganic Nanopores from the Molecular Simulations

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Objectives/Scope:

Geological Carbon Storage (GCS) in depleted tight reservoirs is considered a promising technology for reducing carbon dioxide emissions. These tight reservoirs feature numerous nanoscale pores that provide ample adsorption space for gases. However, the pH values of the reservoir pores vary, and the extended exposure to different pH environments over time can result in distinct surface properties of inorganic nanopores on quartz (pH effects characterized by the deprotonation degree of silanol groups on the quartz surface). This variability may impact the adsorption capacity of gases, but the mechanisms remain unclear. Therefore, a comprehensive understanding of gas adsorption mechanisms, considering reservoir pH values, is crucial for CO₂ sequestration and enhancing methane recovery rates (EGR). This study employs GCMC simulations to investigate the competitive adsorption mechanisms of CO₂/CH₄ in shale inorganic nanopores on quartz, taking into account reservoir pH conditions.

Methods/Procedures/Process:

The adsorption of CO₂, CH₄, and a CO₂:CH₄=1:1 mixture was investigated at reservoir conditions of 353.15K and pressures up to 50MPa. The pH conditions ranged from 2-5, 5-7, to 7-9, corresponding to deprotonation degrees of 0%, 9%, and 18%, respectively. Quartz nanopores, CH₄, and CO₂ were modeled using the CLAFF, TraPPE-UA, and TraPPE-EH models. GCMC simulations were conducted using the MCCCSTowhee software. Each simulation consisted of 2×10⁸ steps in total, with 5×10⁷ steps for equilibration and 1.5×10⁸ steps for statistical sampling. Atomic trajectories were saved every 2000 steps for subsequent data analysis. Using the simulated results, we computed the one-dimensional and two-dimensional density distributions of gases, as well as the excess adsorption. Additionally, we accounted for changes in adsorption phase volumes under three pH environments to calculate the absolute adsorption amounts.

Results/Observations/Conclusions:

The study revealed that with an increase in deprotonation degree, the adsorption phase volumes of CO₂ and CH₄ slightly increased in both single-component and competitive adsorption scenarios. In competitive adsorption, the injection of CO₂ exhibited a more pronounced effect in reducing the adsorption density of CH₄ as the deprotonation degree increased (corresponding increase in pH). In single-component adsorption, both the excess adsorption and absolute adsorption of CO₂ increased with the increasing deprotonation degree, while the impact on CH₄ was minimal. In competitive adsorption, CO₂ significantly decreased the excess adsorption of CH₄, and beyond a pressure of 30MPa, the excess adsorption even became negative. With an increase in deprotonation degree, both the excess adsorption and absolute adsorption of CO₂ increased, while the adsorption of CH₄ slightly decreased. This suggests an enhancement in the competitive adsorption capability of CO₂.

*Applications/Significance/Novelty:

This study provides molecular-level insights into the adsorption behavior of CO₂/CH₄ in quartz nanopores under varying pH conditions. The findings contribute to establishing a theoretical foundation for CO₂ storage and methane recovery enhancement under reservoir conditions with different pH levels.

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