

## Molecular Simulation of Competitive Adsorption of CO<sub>2</sub>-Shale Oil in Kerogen with Different Moisture Content

**Authors :** Shanshan Yang, Zhengfu Ning, Ying Kang

**Abstract :** The competitive adsorption between shale oil and CO<sub>2</sub> in kerogen is of great significance for CO<sub>2</sub> enhanced oil recovery (CO<sub>2</sub>-EOR) and CO<sub>2</sub> storage. In this paper, molecular dynamics (MD) method is used to construct dry kerogen model, and grand canonical Monte Carlo (GCMC) method is used to construct shale reservoir kerogen model with different moisture content. Considering the influence of moisture content and shale oil composition, the competitive adsorption behavior of shale oil and CO<sub>2</sub> in kerogen is simulated, and the feasibility of CO<sub>2</sub> storage was evaluated. The results show that the presence of moisture content significantly reduces the ability of CO<sub>2</sub> to replace shale oil. With the increase of moisture content, the adsorption capacity of shale oil decreases, and the effect of CO<sub>2</sub> replacement of shale oil is improved. The adsorption capacity of long chain alkanes in shale oil decreases under moisture condition, and the competitive adsorption effect between short chain alkanes and CO<sub>2</sub> is more obvious. This study provides an effective guide to quantitatively reveal the competitive adsorption between CO<sub>2</sub> and shale oil from the microscopic perspective.

**Keywords :** competitive adsorption, kerogen, moisture content, shale oil, carbon dioxide, molecular simulation

**Conference Title :** ICAE 2025 : International Conference on Applied Energy

**Conference Location :** Istanbul, Türkiye

**Conference Dates :** May 01-02, 2025