Molecular Simulation of Competitive Adsorption of CO₂-Shale Oil in Kerogen with Different Moisture Content

Authors : Shanshan Yang, Zhengfu Ning, Ying Kang

Abstract : The competitive adsorption between shale oil and CO_2 in kerogen is of great significance for CO_2 enhanced oil recovery (CO_2 -EOR) and CO_2 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_2 in kerogen is simulated, and the feasibility of CO_2 storage was evaluated. The results show that the presence of moisture content significantly reduces the ability of CO_2 to replace shale oil. With the increase of moisture content, the adsorption capacity of shale oil decreases, and the effect of CO_2 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_2 is more obvious. This study provides an effective guide to quantitatively reveal the competitive adsorption between CO_2 and shale oil from the microscopic perspective.

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

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