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MOLECULAR SIMULATION OF CH_4 ADSORPTION AND DIFFUSION IN MONTMORILLONITE

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ABSTRACT This paper established three micro structure models with different basal spacing in montmorillonite, and studied the effect of CO_2 and H_2O to CH_4 adsorption and diffusion. Grand Canonical Monte Carlo (GCMC) and molecule dynamic (MD) simulations were taken to investigate the adsorption and diffusion behaviours of shale gas in montmorillonite at different temperature, pressure and burial depth. The results show that the adsorption quantity of CH_4 increases with the increase of pressure and eventually tends to saturation. The effect of pressure to CH_4 adsorption is more significant than temperature. The adsorption quantity of CH_4 firstly increases with the increase of burial depth, then slightly reduces. The existence of H_2O reduces both the adsorption and diffusion of CH_4, while the existence of CO_2 reduces the adsorption quantity but increases the diffusion coefficient. Therefore, it can be concluded that humid environment is not beneficial to the CH_4 storage and mining, but CO_2 displacement is a good way to the exploitation of shale gas.

Keywords Montmorillonite, Competitive adsorption, Diffusion, Displacement mining