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Dynamic adsorption of CO2 in shale organic pores using molecular dynamic simulation

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The technology of CCUS(carbon capture,utilization and storage) has great potential for development. It is of great significance for CS-ESGR (CO2 sequestration and enhanced shale gas recovery) to study the dynamic adsorption characteristic of CO2 in the organic pore of shale. Most studies analyze the adsorption efficiency and influencing factors at the level of results, while less attention is paid to the phenomena in dynamic processes. In this study, a shale organic pore model consisting of 1 nm and 4 nm micropores connected by 8 nm mesopores is established. And then, the dynamic process of CO2 diffusion from 8 nm mesopores to micropores and adsorption is investigated by using MD(molecular dynamics) simulation method. On this basis, the effects that different pressures on the diffusion of CO2 into micropores with different pore sizes and the adsorption dynamic process are also investigated. It is found that different pore sizes lead to different density distribution, and the dynamic process of diffusion and adsorption occurs in the micropore with pore size of 1 nm at first. This is due to the stronger pore effect of 1 nm micropore, which enhances the adsorption of CO2 with the organic pore surface. At low pressure, the adsorption amount in the 4nm pore is always larger than that in the 1nm pore. At high pressure, the adsorption amount in the 4nm pore is larger than that in the 1nm pore at the initial stage, but it tends to be close to that in the end. In addition, it is beneficial for the faster diffusion of CO2 into the micropore and stronger adsorption with increasing pressure. As a result, the adsorption process fluctuates at a less degree and is more stable at high pressure, the dynamic time to reach adsorption equilibrium is also smaller. It is concluded that pore size has an obvious effect on adsorption at low pressure, which can be explained by spatial constraints and interaction enhancement. While pore size effect gradually diminishes and pressure effect increases at high pressure.

Time Block Preference

Time Block A (09:00-12:00 CET)

References

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