Oil Adsorption Capacity of Clay Minerals in Shale: A Molecular Dynamic Simulation Investigation

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Abstract

Shale oil trapped in a complex network of small pores generally occurs in adsorption and free states. Oil adsorbed on pore surface has weak fluidity, while free oil inside the pore is more movable. Strong adsorption is expected to induce large changes in the phase behavior of hydrocarbons and affects their transport. Thus it is necessary to understand the hydrocarbon adsorption behavior in shales. Some clay minerals (e.g. montmorillonite, kaolinite, and illite) were chosen to study the hydrocarbon adsorption behavior of shales via molecular dynamic simulation, which is a thermodynamic calculation method with molecular movement obeying Newton's laws of motion. Shale oil has complex components; herein, n-C17H36, cyclohexane, methylbenzene, 3-methylpenanthrene, and porphyrin were used for simulation. After each type of hydrocarbon component was separately adsorbed in the slit pore (pore diameter = 9.5 nm) of montmorillonite at 358 K, some molecules adhered to the mineral surface in a multilayered form, whereas some appeared disordered in the pore space. The multilayered portion was in the adsorption state, whereas the disordered section was in the free state. Adsorption layers were 2.6-4.5 nm thick and the thicknesses varied with hydrocarbon components. Distributions of hydrocarbon components in the pores of kaolinite were similar to those in montmorillonite except for n-C17H36. More n-alkane molecules were observed in the free state in kaolinite, indicating that montmorillonite has a stronger hydrocarbon adsorption capacity than kaolinite. Most of the five hydrocarbon components were freely distributed in the pores of illite, suggesting that the illite had a weaker hydrocarbon adsorption capacity. When water (Sw = 30%) and hydrocarbon simultaneously exist, water

layers are distributed on the mineral surface, showing that water are easily adsorbed and can restrain the hydrocarbon adsorption capacity of clay minerals. Some hydrocarbon molecules can pass through the water layer and adsorb close to the mineral surface. Porphyrin exhibited this behavior; however, it was almost invisible in n-$C_{17}H_{36}$ or cyclohexane, indicating that the polarity of the hydrocarbon components had a positive effect on adsorption capacity. Overall, the hydrocarbon adsorption capacity of clay minerals is montmorillonite > kaolinite > illite. Water in pores can restrain this capacity, whereas hydrocarbon polarity can promote it. This study offers a new method for estimating the mobility of shale oil.

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