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Microscopic mechanism of CO₂ huff-n-puff promoting shale oil mobilization in organic/inorganic nanopores

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CO₂ huff-n-puff is a potential promising approach for enhanced recovery and sequestration of CO₂ in shale reservoirs. It is of great practical significance to understand the CO₂ huff-n-puff mechanism from a microscopic point of view. Here, we investigate three stages of CO₂ huff-n-puff promoting shale oil mobilization from organic-inorganic nanopores by molecular dynamics simulation. We show that during the adsorption process of shale oil, due to the presence of active molecules, the adsorption density and strength of shale oil on kaolinite wall are higher than kerogen, but the influence range of shale oil is smaller than kerogen. In the CO₂ soaking stage, although CO₂ has a desorption effect on shale oil near both sides of the wall, stripping shale oil near the inorganic surface was more effective than the kerogen surface. In addition, due to the presence of hydroxyl on the surface, when CO₂ is slightly away from the equilibrium position on the surface of kaolinite, the attraction between CO₂ and kaolinite will become repulsive force under the action of electrostatic force. In the CO₂ puff stage, compared with the ideal model of 0 pressure, when the CO₂ puff pressure is 10MPa, CO₂ can effectively dissociate the "bullet head" structure of the medium component blocking the pore exit through the synergistic effect of miscible phase, viscosity reduction and swelling. Increase overall shale oil recovery by more than 37%. This work first investigates the CO₂ huff-n-puff mobilization of shale oil from multiple stages, and effectively reveal the promoting effects of CO₂ on different components of shale oil in each stage of huff-n-puff.

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