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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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## References

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