

Molecular Simulation of Enhanced Oil Recovery of Shale Oil

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Abstract

A significant amount of oil is trapped within organic nanopores of shale that cannot be recovered by primary production from these resources. The main reason for the large unrecovered oil volumes in shale reservoirs is the presence of nanoscale pore sizes, which leads to extremely small permeability values, and trapping of hydrocarbons in the adsorbed state on the surfaces the pores. For these resources, effective enhanced oil recovery (EOR) techniques are required to displace oil from nanoscale shale matrix. Due to small permeability, it is difficult, if not impossible, to conduct water and chemical flooding in these resources. Maintaining a stable flood front in immiscible gas flooding is challenging due to the severe fingering phenomenon cause by the naturally fractured nature of these formations. Gas huff-n-puff becomes the most suitable EOR method in shale reservoir development. For decades, carbon dioxide EOR techniques have been successfully applied in conventional reservoirs to improve oil production. In this work, the physics behind CO₂ injection into organic nanopores of shale is investigated using molecular dynamics simulations. A 3D kerogen nanochannel, based on the kerogen unit molecules prepared by Ungerer et al. 2014, is created along with a synthetic oil mixture created based on the experimental study of phase behavior of petroleum mixtures performed by Turek et al. (1984). Supercritical CO₂ (sCO₂) is then injected into the channel at different pressures and oil recovery factors are computed. Results of this study demonstrates that the C₇+ component of the oil sample have higher adsorption tendency than lighter hydrocarbon components. Furthermore, it is shown that sCO₂ could potentially produce oil, especially lighter components, from organic matters in shale oil reservoirs. It is observed that as sCO₂ injection

pressure increases, the required soaking time for maximum process performance increases.

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