11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
July 20 - 25, 2014, Barcelona, Spain

Nanofluids for Enhanced Oil Recovery: Molecular Simulations and Mechanism

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Key Words: *Nanofluids, Nanoparticles, Enhanced Oil Recovery, Molecular Dynamics Simulations.*

Nanofluids, which are the term for suspensions of nanometersized structures, have recently been extensively used in a rapidly increasing number of applications, such as enhanced oil recovery (EOR) [1-3]. The presence of nanoparticles alters the wetting properties of nanofluids even at low volume concentrations [4]. However, the nanoparticle interactions with the base fluid and the solid surface bring many challenges in understanding the underlying mechanism. Synthesis of efficient oil recovery agents requires comprehensive studies of the dynamic wetting behavior of nanofluids near the contact line [5].

In this work, we introduced the molecular dynamics (MD) simulation methods to investigate the detachment process of oil droplet immersed in nanoparticle suspension at the nanometer level [6, 7]. We have developed a preprocess program to model the complicated oil-nanofluid-rock system. The oil droplet was modeled as a ternary mixture of toluene, heptane, and decane, respectively. The nanofluid consists of rigid nanoparticles suspended in water.

Contact line radius and contact angle of the oil droplet under various scenarios were calculated as the measure of the degree of detachment. Our MD results show that the performance of the nanofluids in EOR is sensitive to size, volume concentration, and especially the particle charge and the surface properties of the nanoparticles. Nanofluids of hydrophobic nanoparticles show a better performance in oil removal than hydrophilic nanoparticle suspensions, which is consistent with the experimental observations. It is observed that hydrophilic nanoparticles will lead to reduction of the mobility of the nanofluids, which is not good choice for EOR. For hydrophobic nanoparticles, the adsorption on the solid substrate would change the interactions between particles mediated by fluid interfaces near the contact line. Hence the retreat of the contact line and the detachment of the oil droplet will be promoted. We found that the larger volume concentration results in more visible nanoparticle adsorption on solid surface. This effect further induces an advancing displacement of the contact line compared with the meniscus profiles in low concentration case and that with the absence of nanoparticles [6].

More interesting, our simulated results demonstrate a significant enhancement of the oil removal efficiency using nanofluids of charged nanoparticles. When the charge on each particle exceeds a threshold value, the complete detachment of the oil droplet occurs spontaneously [7]. Our MD results also reveal that the dynamic detachment of the oil droplets is sensitive to the charge quantity and the surface wettability of each particle.

Our MD results provide new insights to the effect of nanoparticles for applications in EOR. These findings also provide an optimization opportunity for nanoparticle synthesis by surface coating and surface chemistry techniques. The numerical results can be used to optimize the geometrical and physical parameters of the nanoparticles in the flooding nanofluids, which may provide further support for petroleum industry and environmental improvement activities.

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