Molecular Mechanism of Enhanced Oil Recovery with Nanofluids

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Nanofluids have attracted wide interest in oilfield applications for enhanced oil recovery (EOR). The presence of nanoparticles alters the wetting properties of nanofluids even at low volume concentrations. 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. Our MD results show that the performance of nanofluids in EOR is sensitive to particle charge and surface properties of nanoparticles. It is observed that the presence of the charged nanoparticle can enhance the detachment of oil droplet. For hydrophobic nanoparticles, the retreat of the contact line and the detachment process will be promoted. These studies can provide new insights to the effect of nanoparticles for applications in EOR. The numerical results can be used to optimize the geometrical and physical parameters of the nanoparticles in the flooding nanofluids.

**Keywords:** Nanofluids, Enhanced oil recovery, liquid solid interface, charge, Molecular dynamics