World Academy of Science, Engineering and Technology
International Journal of Chemical and Materials Engineering
Vol:15, No:05, 2021

Atomistic Insight into the System of Trapped Oil Droplet/ Nanofluid System in Nanochannels

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Abstract : The role of nanoparticles (NPs) in enhanced oil recovery (EOR) is being increasingly emphasized. In this study, the motion of NPs and local stress distribution of tapped oil droplet/nanofluid in nanochannels are studied with coarse-grained modeling and molecular dynamic simulations. The results illustrate three motion patterns for NPs: hydrophilic NPs are more likely to adsorb on the channel and stay near the three-phase contact areas, hydrophobic NPs move inside the oil droplet as clusters and more mixed NPs are trapped at the oil-water interface. NPs in each pattern affect the flow of fluid and the interfacial thickness to various degrees. Based on the calculation of atomistic stress, the characteristic that the higher value of stress occurs at the place where NPs aggregate can be obtained. Different occurrence patterns correspond to specific local stress distribution. Significantly, in the three-phase contact area for hydrophilic NPs, the local stress distribution close to the pattern of structural disjoining pressure is observed, which proves the existence of structural disjoining pressure in molecular dynamics simulation for the first time. Our results guide the design and screen of NPs for EOR and provide a basic understanding of nanofluid applications.

Keywords : local stress distribution, nanoparticles, enhanced oil recovery, molecular dynamics simulation, trapped oil droplet, structural disjoining pressure
Conference Title : ICNNMR 2021 : International Conference on Nanotechnology, Nanoscale and Microscale Research
Conference Location : Vancouver, Canada
Conference Dates : May 20-21, 2021