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Micro-Scale Simulation and Characterization of Adsorption-Diffusion Behaviors of Nanoparticles onto Mobile Oil/Water Interface

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A novel, hybrid pore-scale simulation method using Lattice-Boltzmann (LB) coupled with Langevin-Dynamics (LD) is proposed to investigate the physics of nanoparticles onto oil/water interface. Based on the LB method, the high-resolution characterization of oil-water two-phase interface is established, independent of further adjustment of interfacial tension (IFT), density and viscosity ratio. Then, in a fashion of discrete LB forcing source distribution, LD method is introduced to characterize the effects of Brownian motion, thermal fluctuation dissipation, multi-body hydrodynamics and particle-particle interactions. The new method is verified using the classical examples including Poiseuille flow velocity distribution calculation, wall wettability, Laplace equation, and the momentum decline of single nanoparticle. By the means of the new LB-LD coupling model, the adsorption and diffusion characterization of nanoparticles onto oil/water interface are investigated.
Moreover, by introducing the interference coefficient and non-equilibrium time, a modified Langmuir adsorption equation is first established by more accurately quantifying the adsorption characterization of nanoparticles and the consequent impacts onto the oil/water interfacial force, of which the classical Langmuir adsorption equation cannot take account. In addition, both the lateral and longitudinal diffusion coefficients of nanoparticles into the water phase and onto oil/water interface are obtained, and of which the underlying mechanisms are explained in detail. The correlation among the primary controlling factors including concentration, size and adsorption-diffusion of nanoparticles is well established. For a target representative example of SiO2 nanoparticles, it is observed that small size nanofluids with high concentration could accelerate the adsorption of nanoparticles and therefore help decrease oil/water interface tension. Attributed to the contributions of non-uniform flow field and curving effects of oil/water interface, the diffusion rates of nanoparticles onto oil/water interface are found as an exponential function of nanoparticle size. The novel simulation and characterization method provide valuable insights into how nanoparticles adsorb and diffuse onto oil/water interface that help reduce oil/water interface tension.

Participation

In-Person

References

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