Contribution ID: **438** Type: **Poster Presentation**

Microscopic Simulation Methods for the Movement and Effects of Nanoparticles at the Oil-Water Interface

Wednesday, 15 May 2024 09:25 (1h 30m)

Nanoparticles are widely used in biomedicine, nanoelectronics, energy devices, and Enhancing Oil Recovery (EOR) due to their unique thermodynamic properties and large specific surface area. Recent research highlights the significant impact of the adsorption and diffusion behavior of nanoparticles at the oil-water interface on interfacial properties, particularly interfacial tension. This suggests that nanoparticles hold the potential to become pivotal materials for altering the permeability characteristics of oil-water flow within porous media. The lattice Boltzmann (LB) method emerges as a powerful mesoscale simulation technique for accurately modeling multiphase flows. In this method, the color gradient model, precisely characterizing parameters such as contact angles and interfacial tension, enables the accurate simulation of oil-water biphasic systems. The Langevin-Dynamics (LD) method excels in providing a detailed force-based characterization of nanoparticles in fluids, encompassing electrostatic forces, van der Waals forces, stochastic forces, and frictional forces. This methodology facilitates the microscale simulation of particle dynamics with a comprehensive understanding of the forces acting on nanoparticles in fluid environments.

A pioneering hybrid pore-scale simulation methodology was firstly introduced for the simulation of movement of nanoparticles and oil-water, employing the integration of Lattice-Boltzmann (LB) with Langevin-Dynamics (LD) for an in-depth exploration of the interactions involving nanoparticles at the oil-water interface. Leveraging the LB method, a high-resolution portrayal of the oil-water interface is established. Subsequently, through a discrete distribution of LB forcing sources, the LD method is incorporated to capture the influences of Brownian motion, thermal fluctuation-dissipation, multi-body hydrodynamics, and particle-particle interactions.

The simulation results indicate that the diffusion and adsorption behavior of nanoparticles at the oil-water interface significantly influences the interfacial tension. The results indicate that the diffusion rate of nanoparticles in a single phase (aqueous phase) is 4 to 6 times higher than the diffusion efficiency at the interface. As the particle size decreases according to a power-law, the diffusion coefficient of nanoparticles increases according to a power-law. This implies that nanoparticles with smaller particle diameters exhibit higher mobility and are more prone to move and adsorb at the oil-water interface. Based on these findings, we firstly propose a modified Langmuir adsorption equation, adjusted for particle non-equilibrium adsorption times (τe), to characterize the impact of nanoparticles on the interfacial tension at the oil-water interface. The equation can depict the real-time variation of the oil-water interfacial tension with increasing adsorption time. Compared to the conventional Langmuir adsorption equation, the computational accuracy is improved by approximately 15%. Finally, we observed the influence of SiO2 nanoparticles and NM4 (with four dodecyl chains uniformly modified on one side) nanoparticles on the oil-water interfacial tension under different particle sizes and injection concentrations. It was found that NM4 exhibited a 1.45 times greater reduction in interfacial tension compared to SiO2 nanoparticles. Meanwhile, small-sized (15 nm) and high concentration (0.08 wt%) of SiO2 nanoparticles have a more pronounced effect in reducing interfacial tension from 24.0 mn/m to 14.1 mn/m.

Acceptance of the Terms & Conditions

Click here to agree

Student Awards

Country

中国

Porous Media & Biology Focused Abstracts

References

Conference Proceedings

I am interested in having my paper published in the proceedings.

Primary author: KE, Can

Co-authors: Prof. YUAN, Bin (China University of Petroleum (Huadong)); Prof. ZHANG, Wei (China University of Petroleum (Huadong)); Mr LI, Yue (China University of Petroleum (Huadong))

Presenter: KE, Can

Session Classification: Poster

Track Classification: (MS23) Interfaces, interfaces everywhere…a special session in honor of Prof. Dorthe Wildenschild