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Nanoscale interface dynamics: Self-assembly and stability of interface film of multi-phase flow in porous media

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Self-assembly phenomena have been observed widely in the interface of multi-phase flow in porous media. Surfactant or surfactant-like particles play an important role during the self-assembly process. In this work, we employed a series of molecular dynamics simulations to investigate the self-micro emulsification and formation of self-assembly nanoparticle film. Atomistic insights into the self-micro emulsifying process and the underlying mechanisms are crucial for the design and tuning of the size of microemulsion droplets toward applications. Coarse-grained models were used to explore the role that droplet sizes played in the preliminary self-micro emulsifying process. The time evolution of liquid mixtures consisting of several hundreds of water/surfactant/oil droplets was resolved in large-scale simulations. By monitoring the size variation of the microemulsion droplets in the self-micro emulsifying process, the dynamics of diameter distribution of water/surfactant/oil droplets were studied. The underlying mass transport mechanisms responsible for droplet size evolution and stability were elucidated. Specifically, temperature effects on the droplet size were clarified. As a continuous task, the self-assembly behavior of amphiphilic nanoparticles was studied, and the mechanical properties of the interface film has been measured. This work provides knowledge of the self-micro emulsification of water-in-oil microemulsions at the nanoscale and the formation of nanoparticles film. The results are expected to serve as guidelines for practical strategies for preparing a microemulsion system with desirable droplet sizes and an expected interface film consisting of nanoparticles.

Participation

In-Person

References

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