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Using dissipative particle dynamics for modeling surfactants

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ABSTRACT

Oil recovery is an industrial process that injects aqueous solutions into an oil reservoir to pump out crude oil and promote the oil production. The aqueous solution contains surfactants for reducing the interfacial tension (IFT) between aqueous phase and oil. The critical micelle concentration (CMC) is the concentration of surfactant above which micelles form and the interfacial tension reaches a plateau. Our research seeks to measure IFT and CMC for surfactants using dissipative particle dynamics (DPD) technique, which is a coarse-grained method based on the molecular dynamics. We first study how IFT is influenced by the surfactant concentration. Furthermore, another simulation is performed, in which an oil drop passes through porous media in the presence of surfactants under various capillary numbers. Using the simulation of emulsion flow through porous media, we get qualitatively similar velocity profile and average velocity as the results from computational fluid dynamics. In addition, the porous media simulation indicates that the presence of surfactants would slightly reduce the average velocity of the oil drop.

KEYWORDS

Surfactant, Dissipative Particle Dynamics, molecular dynamics