Molecular Dynamics Study on the Film Drainage in Water-in-Oil Systems

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Coalescence of water droplets dispersed in a crude oil is an important process in the chemical engineering and petroleum industry. Despite being extensively studied, the process of coalescence is still not completely understood. Particularly, the intermolecular interactions between the complex molecular structures of adsorbed crude oil components (asphaltenes, resins, etc) have a strong effect on the disjoining pressure and can be a significant factor that controls the the stability of the emulsion and may hinder the drop-drop coalescence. However, when developing process models for crude oil systems, only the bulk properties of the crude oil, such as density, viscosity etc. are accounted in most models and the specific chemical footprint (e.g., asphaltene/resin content) of the crude oil is often neglected. On the other hand, numerous laboratory experiments have been performed to study the interfacial phenomena for crude oil-water systems since different interfacially active compounds in the crude oil affect the behavior in these complex systems. Therefore, with the current work we aim to close the apparent gap between crude oil chemical characterization and process modelling of crude oil-water systems. The main objective is to obtain a new semi-empirical expression for the coalescence time that takes into account a general description of the chemical footprint of the crude oil. The first step in this task is to simulate the disjoining pressure at liquid-liquid interfaces for various interfacial concentrations of model asphaltene and resin molecules with molecular dynamics (MD). The MD simulations presented here can be used to estimate the disjoining pressure in a thin liquid film between two drops as a function of the thin film thickness for different interfacial concentrations of surface active compounds indigenous to crude oil. The disjoining pressure is often problematic to be obtained from molecular simulations for liquid-liquid systems. Thus, we employ a new methodology to calculate the disjoining pressure from MD simulations for various film thicknesses and interfacial concentrations of asphaltene molecules at an oil-water interface. The resulting functional behaviors for the disjoining pressure can be subsequently employed in continuum film drainage models to solve for the coalescence time with the interfacial concentration of adsorbed molecules as a parameter.

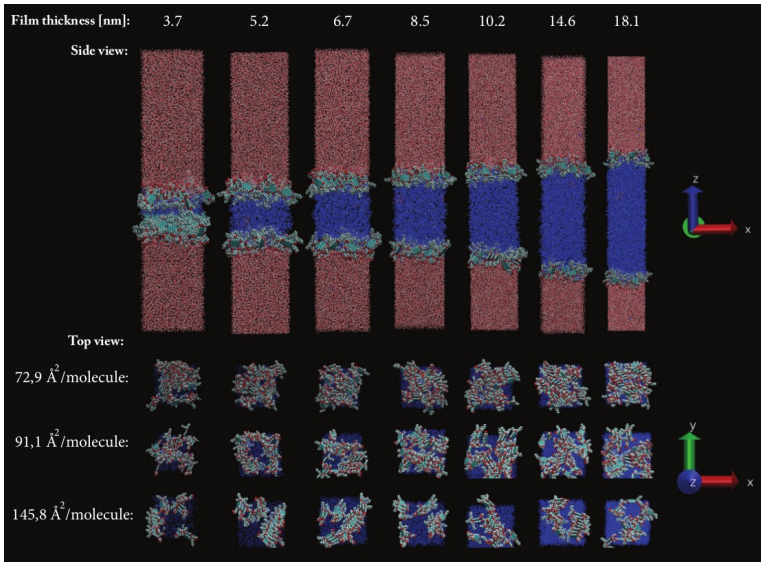

Figure 1 Molecular dynamics simulation on the process of film thinning in water-in-oil system in the presence of asphaltene molecules.