

A numerical vinaigrette: effect of surfactants on oil-water emulsification

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Emulsions are of primary interest in modern engineering research given their heavy usage both in our daily life (e.g., food and cosmetics) and in high-end industrial applications (e.g., drug development). The addition of surfactants, either as additives or contaminants, can affect both the mixing performance and final quality of the mixed product. Therefore, understanding and accurately predicting the outcome of such a scenario is very important, as it facilitates rapid optimisation of the process. In this study, we consider two immiscible liquids, oil and water, stirred by a pitched blade turbine (PBT) in a cylindrical vessel. We investigate the effect of impeller speeds (that leads to the Reynolds number in the range $Re = 5663 - 56632$) and the presence of soluble surfactants. Massively-parallel three-dimensional simulations combined with our high-fidelity hybrid front-tracking level-set interface capturing algorithm [1] are employed to capture the flow dynamics and interfacial behaviours. In the absence of surfactants, the rotation of the impeller introduces a primary vortex (reported previously in the literature for idealised rotational flows), as well as several secondary vortical structures resembling wall-end vortices, vortex breakdown, blade-tip vortices, and Moffatt vortices. These structures lead to lifting of the water phase around the vessel wall, while the oil in the centre is pulled downwards, resulting in a deformed interface with a helical shape composed of four rotating curtains. As the rotational frequency increases, the interfacial deformation is accelerated, producing ligaments which subsequently break into small droplets. For very high rotational speeds, the flow becomes extremely complex with a multitude of interfacial singularities: atomization, creation of ligaments, breakage and coalescence of drops, all occurring simultaneously. The addition of surfactants lowers the local interfacial tension and also generates interfacial surfactant concentration gradients that give rise to Marangoni stresses. We study the effect of these stresses on the mechanisms and flow phenomena accompanying the mixing process by exploring various values of surfactant elasticity and the Biot number. By analysing the drop size distribution at steady state for both surfactant-free and surfactant-laden system, we highlight the fact that higher impeller speeds lead to a larger number of dispersed drops until drop coalescence dominates breakage; the presence of surfactant is associated with interfacial rigidification, suppression of end-pinching, and promotion of tip-streaming.

REFERENCES

- [1] Shin, S. et al. A hybrid interface tracking - level set technique for multiphase flow with soluble surfactant. *J. Comp. Physics* **359**: 409–435 (2018).