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# Direct numerical simulation of the dispersion dynamics of complex flows in static mixers

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Mixing is a fundamental operation in most modern industrial processes, occurring in a vast array of applications. In particular, mixing of immiscible liquid-liquid systems is of primary interest given their heavy involvement both in consumer goods and in high-end industrial applications. Given the intrinsic complexity behind these systems, design and scale-up methodologies are largely dependant on limited empirical models, which has led to over-design practices to guarantee a minimum level of quality and performance, hence compensating for the lack of fundamental knowledge of the process. This project aims to provide a deeper understanding of the complex underlying physical mechanisms governing immiscible liquid-liquid mixing. This study focuses on static mixers that have been shown to be a promising alternative to conventional stirred vessels, handling different inlet configurations and surfactant laden flows, which are common yet complex scenarios encountered in several industrial applications.

We implement massively-parallel, high-fidelity, three-dimensional direct numerical simulations with a state-of-the-art code which is based on a hybrid front-tracking level-set interface capturing algorithm. This hybrid formulation provides a wealth of information and flexibility previously unavailable, which allows us to account, in detail, for complex interfacial phenomena in industrially relevant scenarios. In this study, we consider three cases for the initial configuration of the dispersed phase: 1) isolated cases, individual droplets, mimicking a controlled syringe injection; 2) multiple droplets with different sizes simulating a pre-dispersed inlet; and 3) a jet inlet, emulating a standard phase injection from a gear pump. Furthermore, we explore surfactant-laden flows, for some of the configurations mentioned above, with varying properties which are modified through parameters such as surfactant elasticity, diffusivity, among others. The simulations elucidate a two-step breakup mechanism occurring in the static mixer, consisting of an initial elongational deformation with no breakup, mostly driven by buoyant forces, followed by a ligament stretching which results in pinch-off, giving birth to smaller daughter droplets. The first step is mostly dominated by high stretching efficiencies, whilst the second step features a periodic variation of stretching and squeezing flows causing the pinch-off. In addition, the surfactant-laden simulations have demonstrated that ligament pinch-offs tend to be suppressed, following a rigidification of the interface as a result of the dominating Marangoni stresses over the inertial forces. This alters substantially the deformation and breakup mechanism identified for the "clean" cases.