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Effect of surfactants on the flow dynamics of liquid drops in complex microchannel geometries

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The motion of drops in the presence of an immiscible continuous liquid phase in microchannels is an increasingly relevant process in a vast array of applications, including those related to the medical field, the production of pharmaceuticals, and the oil & gas industry. Surface-active agents as undesirable contaminants or deliberately-placed additives are pervasive in these applications and have been shown to influence various flow parameters and induce Marangoni phenomena. In this study, the surfactant-laden drop formation and flow dynamics of 3-D liquid-liquid flow in a microfluidic device have been simulated through a hybrid front-tracking/level-set computational code in a highly-parallel framework. The geometry of the microchannel simulated is characterised by a number of complexities, such as an intricate narrowing junction for fine-tuned drop formation and a planar-shaped cross-section for the inlets and outlet. The non-ideal and non-symmetric attributes of this channel introduce additional flow features when compared to simple channels with purely circular or square cross-sections [1]. The construction of this geometry was based on a static distance function, several primitive objects (e.g., cylinders, planes, and torii), and simple operations between them. The validated simulations elucidated the three main stages of drop formation in the dripping regime: expansion, necking, and pinch-off. The impact of soluble ionic and anionic surfactants at different concentrations was examined in terms of drop size, formation time, and velocity distributions within the drop. It was found that the presence of surfactants tends to lower the droplet size and formation time due to decreased interfacial tension, as well as suppress the large re-circulation zones typically found in 'clean' cases. Finally, the distribution of surfactant concentration across the interface, and its close relationship with Marangoni stresses and flow parameters of the drop, were thoroughly analysed in the system.

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