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Multi-phase simulations of ultra-low interfacial tension all-aqueous droplets in microfluidics

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ABSTRACT

Microfluidics is the study of fluid flows at micrometer length scales, with fundamental significance and diverse applications in many important fields such as drug delivery, cell/microorganism encapsulation, environmental monitoring, and Green Energy. Droplet microfluidics involves the controlled generation of droplets inside microfluidic devices, where two immiscible liquid phases interact. This can be conducted in a T-junction or flow-focusing device, where a dispersed (inner) phase, injected along the main channel, is fragmented by a continuous (outer) phase. In general, droplet formation in microfluidic devices is a complex phenomenon that depends on the material properties of the phases involved (such as their viscosities and interfacial tension), flow parameters (such as the flow rate of either phase and the geometry of the microfluidic device), and natural instabilities that occur at the interface.

In an Aqueous Two-Phase System (ATPS), immiscible liquid phases are formed by the phase separation of two incompatible solvents in water. The most widely studied ATPS is formed by dissolving the polymers poly (ethylene glycol) (PEG) and dextran (DEX) in water. Upon reaching thermodynamic equilibrium, the system separates into a PEG-rich and DEX-rich phase. Polymeric ATPS is highly biocompatible, which makes it an advantageous candidate for biomedical applications. However, the system also has an ultra-low interfacial tension (1-100 µN.m), making it challenging to study experimentally produced droplet behavior methodically. Hence, a method is required to systematically control flow parameters and study their effect on the physics of ATPS droplet formation.

In this study, Volume-of-Fluid (VOF) Computational Fluid Dynamics (CFD) simulations are conducted on ANSYS Fluent to investigate the underlying physics of ATPS droplet formation in microfluidic devices. Notably, the Pressure Implicit with Splitting Operators (PISO) and the Geo-Reconstruct method are used for pressure-velocity coupling and interface capture, respectively. The computational domain, boundary conditions, and material properties are based on our in-house experiments, where DEX-in-PEG droplets are passively generated within poly (dimethyl siloxane) (PDMS) microfluidic devices. Preliminary results show good qualitative agreement between experimental and numerical results. Our immediate findings demonstrate the transitioning between flow regimes when key parameters such as flow rate ratio and capillary number are systematically varied. Numerical simulations quantitatively classify the dripping-to-jetting transition regimes observed in the experiments. Our study aims to develop innovative methods for controlled ATPS droplet production, bringing them closer to point-of-care and commercial viability.