Lattice Boltzmann Simulation of Droplet Generation in a Microfluidic Cross-Junction

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Abstract. Using the lattice Boltzmann multiphase model, numerical simulations have been performed to understand the dynamics of droplet formation in a microfluidic cross-junction. The influence of capillary number, flow rate ratio, viscosity ratio, and viscosity of the continuous phase on droplet formation has been systematically studied over a wide range of capillary numbers. Two different regimes, namely the squeezing-like regime and the dripping regime, are clearly identified with the transition occurring at a critical capillary number Ca_{cr}. Generally, large flow rate ratio is expected to produce big droplets, while increasing capillary number will reduce droplet size. In the squeezing-like regime ($Ca \leq Ca_{cr}$), droplet breakup process is dominated by the squeezing pressure and the viscous force; while in the dripping regime ($Ca > Ca_{cr}$), the viscous force is dominant and the droplet size becomes independent of the flow rate ratio as the capillary number increases. In addition, the droplet size weakly depends on the viscosity ratio in both regimes and decreases when the viscosity of the continuous phase increases. Finally, a scaling law is established to predict the droplet size.

1 Introduction

Rapid development of microfabrication technologies has facilitated a broad range of microfluidic applications especially in biology and chemistry. Microdroplet technology has recently emerged as a promising flexible platform for microfluidic functions [1–3] where a droplet acts as an individual chemical reactor. As samples/reagents are confined in the

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droplets, it can avoid sample/surface interaction and thus eliminate surface adsorption and cross sample contamination. The miniaturization of the entire process can enable the rapid analysis of very small quantities of droplet samples in a portable, automated and inexpensive format [4]. Many microfluidic devices have emerged to generate uniform droplets, including geometry-dominated devices [5, 6], flow-focusing devices [7–10], *T*-junctions [11–16] and co-flowing devices [17, 18].

Although flow physics of droplet generation at *T*-junctions has been extensively investigated both experimentally and numerically, significant effort is required to understand droplet generation in a confined cross-junction. The droplet dynamics in a microfluidic cross-junction is very complicated. Many coupled factors will affect the droplet formation process, e.g., interfacial tension, wetting properties and confinement of flow channels, fluid flow rates and viscosities. Cubaud et al. [8] investigated the liquid/gas flows in a cross-junction and found that the bubble breakup could be understood as the competition between the pressure drops in the liquid and gas phases. The bubble size could be predicted by the gas/liquid flow rate ratio. Garstecki et al. [9] investigated the mechanism for bubble breakup process in the cross-junction with a small orifice, and observed that the collapsing rate of the neck is quasi-stationary and proportional to the liquid flow rate. Tan et al. [19] studied the formation mechanism of plug flow in an oil/water microfluidic cross-junction. They found that the plug size depends on the flow rate ratio of both fluids and the capillary number. Recently, Fu et al. [10] found that the bubble (slug) breakup process in a cross-junction is mainly controlled by the collapse stage, during which the collapse rate of the thread neck and the collapse time were affected by the gas/liquid flow rate ratio and the viscosity of the liquid phase. Although the experimental studies have helped to understand the underlying physics, the current available data are sporadic. Various materials were used to fabricate the microchannels with a diverse range of dimensions, and the experiments are operated under a wide range of flow conditions with different fluids. Consequently, the information is fragmented, which leads to inconclusive and even incompatible findings. On the other hand, experiments at such small scales are still difficult. For example, it is challenging to accurately measure droplet size, pressure and velocity fields, and droplet deformation, breakup, and coalescence. Numerical studies are therefore essential for understanding droplet dynamics, complementary to experimental investigations.

Davidson et al. [20] used volume of fluid (VOF) method to predict the dynamics of droplet formation in an axisymmetric microfluidic flow-focusing geometry. The ending pinching and capillary-wave instability were found to be important for droplet breakup from the liquid jet with high flow rate. Hua et al. [18] used front-tracking/finite volume method to investigate the mechanism of droplet formation in a coflowing microchannel. The effects of the continuous phase flow rate, viscosity, and the interfacial tension on the droplet size were investigated in both dripping and jetting regimes, where the correlations of droplet size and Reynolds number, Weber number, capillary number, and viscosity ratio were obtained respectively. The lattice Boltzmann method (LBM) has shown great potential to model the interfacial interactions while incorporates fluid flow as a