

NUMERICAL INVESTIGATIONS OF LIQUID-LIQUID FLOWS THROUGH MICROCHANNELS

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Summary

Liquid-liquid flows in microchannels are important to microreactors/ microfluidic devices that are used to carry of liquid-liquid reactions, extractions, emulsifications etc. In this work, we report numerical investigations of drop/slug formation and flow regimes for liquid-liquid (oil-water) flow in micro-channels. The Volume-of-Fluid (VOF) method was used to simulate the dynamics of water drop/slug formation in silicone oil and predicted drop/slug shapes/lengths were compared with the measurements of Garstecki et al. [1]. The effects of flow rates of water and oil phases (0.019 - 0.417 $\mu\text{L/s}$ and 0.004 - 0.14 $\mu\text{L/s}$, respectively), channel size, liquid-liquid distributor (T-junction and Y-junction) and liquid viscosity on liquid-liquid flow regimes and slug lengths, were investigated. The predicted drop/slug formation dynamics/slug lengths agreed the measurements of Garstecki et al. [1] satisfactorily for ratio of flow rates ($Q_{\text{water}}/Q_{\text{oil}}$) in the range of 0.1-1.7. However, for $Q_{\text{water}}/Q_{\text{oil}} > 1.7$, unlike the (long) slug flow reported by Garstecki et al. [1], a parallel flow was observed in the numerical simulations. The effect of wall adhesion (contact angle) on the flow regimes and slug lengths was also investigated. The experimentally validated computational model will be useful to simulate mixing, transport processes and chemical reactions in microchannels.

Keywords:

Microchannel, Liquid-liquid flows, Simulation, Drop, Slug, Volume of fluid method

Introduction

Microreactors offer high surface to volume ratio and small diffusion paths than the conventional reactors. Since heat and mass transfer rates are enhanced; exothermic, fast reactions can be carried out in micro-reactors with better yield, selectivity and control. Micro-reactors involving liquid-liquid two-phase flows in micro-channels are important for several chemical processing applications, for example, liquid-liquid extractions, emulsifications, nitration and hydrogenation reactions etc. It is therefore important to understand the hydrodynamics of liquid-liquid flows through microchannels.

Several experimental investigations were carried out to understand the effects of flow rates of liquid phases, liquid viscosity and interfacial tension, liquid distributor and channel configuration on flow regimes and drop/slug size/length. Garstecki et al. [1] studied formation of drops/slugs in a microfluidic T-junction channel for oil-water system and proposed the scaling law $L/W_{\text{oil}} = 1 + \alpha (Q_{\text{water}}/Q_{\text{oil}})$ to predict the slug length.

The accuracy and range of applicability of the scaling law was verified experimentally for different $Q_{\text{water}}/Q_{\text{oil}}$ (0.1 - 10), μ_{oil} (0.01-0.1 kg/m.s), surface tension and channel configurations. Kashid et al. [2] investigated the effects of various operating conditions on the flow regimes, slug size, interfacial area and pressure drop for liquid-liquid flows in Y-junction capillaries. Zhao et al. [3] experimentally studied the liquid-liquid flow regimes in a microchannel viz. mono-dispersed drop flow, slug flow, parallel flow based on the Weber numbers of fluid phases.

Kashid et al. [4] studied the slug flow in the Y-junction microchannel numerically and concluded that the surface tension and wall adhesion plays an important role in the slug generation. The objective of the present work was to verify the predictive capabilities of the VOF method to simulate various liquid-liquid flow regimes observed experimentally and to predict the drop/slug shapes/lengths for a wide range of flow rates of the liquid phases; fluid properties (viscosity and interfacial tension), distributor geometry and channel size using the measurements of Garstecki et al. [1].

Results and Discussion

Numerical simulations of liquid-liquid flows in a T-junction micro-channel were performed using the VOF method implemented in the commercial solver FLUENT v6.3 (of Ansys Inc, USA). The silicone oil and water were considered as the working fluids ($\rho_{\text{oil}} = 930 \text{ kg/m}^3$, $\rho_{\text{water}} = 1000 \text{ kg/m}^3$, $\sigma_{\text{oil-water}} = 0.0365 \text{ N/m}$, $\mu_{\text{oil}} = 0.01 \text{ kg/m.s}$, $\mu_{\text{water}} = 0.001 \text{ kg/m.s}$) The simulations were performed for Q_{oil} in the range of 0.01-1 $\mu\text{L/s}$ and Q_{water} in the range of 0.004 - 0.14 $\mu\text{L/s}$ (the corresponding $Q_{\text{water}}/Q_{\text{oil}}$ was in the range 0.1-1.7), for widths of the water inlet (W_{water}) and oil inlets (W_{oil}) in the range of 50 - 100 μm and height of channel (H) in the range of 33 - 79 μm . The effect of inlet distributor was investigated by considering a T-junction and Y-junction micro-channel. The predicted and experimental slug formation mechanism and slug lengths were in a satisfactory agreement with the measurements of Garstecki et al. [1] for $Q_{\text{water}}/Q_{\text{oil}} < 1.7$ as shown in Figure 1. The drop/slug flow regimes for superficial velocities (of

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water) in the range 0.001-0.1 m/s simulations could be satisfactorily predicted as shown in Figure 2. The effect of μ_{oil} was investigated at two values of viscosities (0.01 kg/m.s and 0.1 kg/m.s) and there was no significant change in slug lengths for these two values of viscosities. The effect of channel size on the slug length was simulated for three different geometries of T-junction (a) $W_{oil} = 100 \mu\text{m}$, $W_{water} = 50 \mu\text{m}$, $H = 33 \mu\text{m}$, (b) $W_{oil} = 100 \mu\text{m}$, $W_{water} = 100 \mu\text{m}$, $H = 33 \mu\text{m}$ (c) $W_{oil} = 50 \mu\text{m}$, $W_{water} = 50 \mu\text{m}$, $H = 33 \mu\text{m}$ for Q_{water}/Q_{oil} in the range of 0.15-2.0 as shown in Figure 3. For $Q_{water}/Q_{oil} < 1$, it was observed that the predicted L/W_{oil} were in $\pm 20\%$ of the measured L/W_{oil} (see Figure 3). For $Q_{water}/Q_{oil} > 1$, either the slug length were significantly over predicted or a parallel flow was observed than the slug flow regime observed experimentally.

The simulations were performed to investigate the effect of distributor geometry (different configurations of T-junction, Y-junction) having dimensions of $W_{oil} = 100 \mu\text{m}$, $W_{water} = 100 \mu\text{m}$, $H = 33 \mu\text{m}$ for different flow rate ratios ($Q_{water}/Q_{oil} < 1$). It was observed that for the same flow rate ratio, the slug lengths were larger for Y-junction than that observed for the T-junction microchannel. With the increase in the three-phase contact angle, it was also observed that parallel flow changes to slug flow. Detailed results on the effect of wall contact angle on the flow regimes and drop/slug length will be presented in the full manuscript. Further details of the effects of width of oil and water inlets, height of channel and type of distributor on the flow regimes, drop/slug formation mechanism and drop/slug lengths will be reported in the full length manuscript. The experimentally validated computational model will be useful to simulate mixing and mass/heat transport and to evolve new reactor configurations.

References

- [1] Garstecki, P.; Fuerstman, M. J.; Stone, H. A.; Whitesides, G. M. Formation of droplets and bubbles in a microfluidic T-junction-scaling and mechanism of break-up, *Lab Chip*, **2006**, 6, 437–446.
- [2] Kashid, M. N.; Agar, D. W. Hydrodynamics of liquid-liquid slug flow capillary micro reactor: Flow regimes, slug size and pressure drop, *Chemical Engineering Journal* **2007**, 113, 1–13.
- [3] Zhao, Y.; Chen, G.; Yuan, Q. Liquid-Liquid Two-Phase Flow Patterns in a Rectangular Microchannel, *AIChE Journal* **2006**, 52, 12, 4052-4060.
- [4] Khasid, M. N.; Platte, F.; Agar, W.; Turek, S. Computational modeling of slug flow in a capillary microreactor, *Journal of Computational and Applied Mathematics* **2007**, 203, 487 – 497.

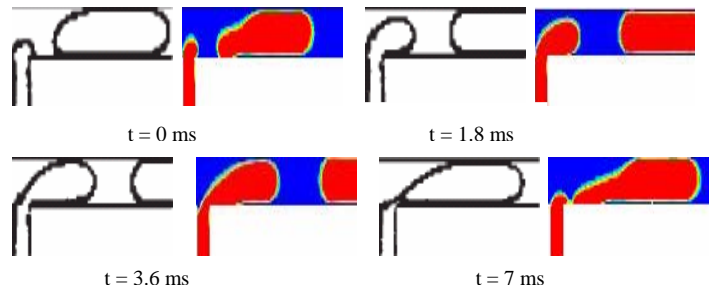


Figure 1. Dynamics of slug formation: Comparison of experimental (Garstecki et al. [1]) and simulated slug shapes ($U_{water} = 0.0848 \text{ m/s}$, $U_{oil} = 0.0252 \text{ m/s}$, $W_{water} = 50 \mu\text{m}$, $W_{oil} = 100 \mu\text{m}$, $H = 33 \mu\text{m}$).

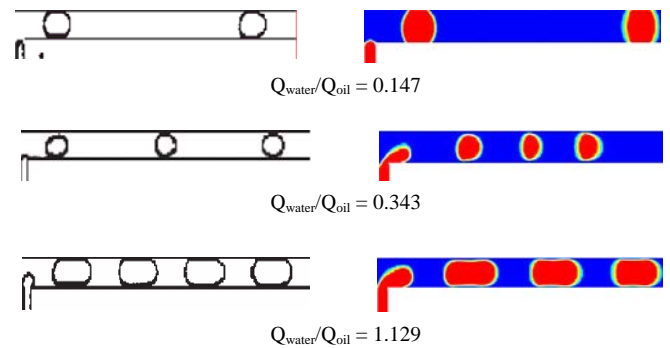


Figure 2. Effect of flow rate on simulated (present work) and experimental (Garstecki et al. [1]) flow regimes ($W_{water} = 50 \mu\text{m}$, $W_{oil} = 100 \mu\text{m}$, $H = 33 \mu\text{m}$, $\theta = 140^\circ$).

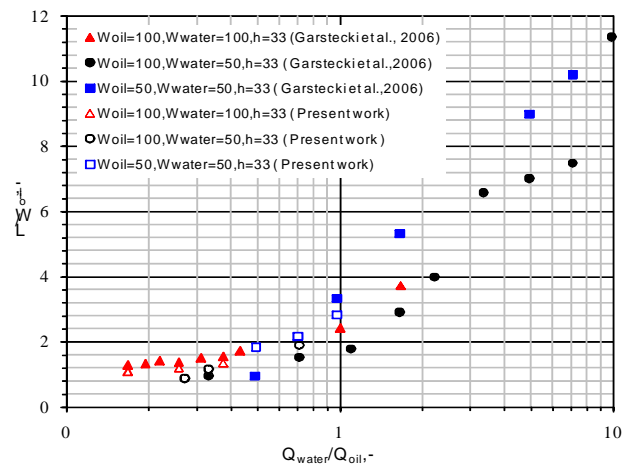


Figure 3. Effect of channel size and T-junction geometry on measured (Garstecki et al. [1]) and simulated (present work) slug lengths.