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EXPERIMENTAL AND NUMERICAL STUDIES OF EMULSION FORMATION IN A MICROFLUIDC T-JUNCTION

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SUMMARY

The production of water-in-oil (w/o) emulsions in T-junction microfluidic channels was studied through experiments and computational fluid dynamics (CFD). w/o emulsions were produced in the microchannels from deionised water and mineral oil. The interfacial tension of the system was controlled to ~ 0.003 N/m using oil-soluble surface active agent (surfactant). A 2-dimensional (2D) CFD model was setup for simulation of the generation of w/o emulsion in a 200μm wide T-junction microchannel. COMSOL Multiphysics, a program based on the finite element method (FEM) was used. The fluid-fluid interface was modelled using the conservative level set method (LSM), where the oil-water interface was implicitly represented by level set function, φ. The simulated droplets differed in size from the droplets observed in experiments. The deviation between the CFD model and experiments was attributed to modelling approach which excluded the variations in contact angle between the two fluids and the channel surface which occur in experimental conditions.

Keywords: Emulsification, emulsion, microfluidics, microchannels, monodisperse, microtechnologies, modelling and simulation, computational fluid dynamics, CFD.

1. INTRODUCTION

The main objective of this work was study the formation of water-in-oil (w/o) droplets in T-junction microchannels using experiments and computational fluid dynamics (CFD) modelling. Microfluidic techniques are currently receiving increased attention as potential substitutes for conventional methods of producing emulsions such as high speed blenders and colloid mills. Many of the applications of emulsions require small size distribution or monodispersity of the droplets in the emulsion. The precision offered by microfluidic methods enables better control for the monodispersity emulsions [1]. Microfluidic systems are also advantageous to lower shear environment and better energy efficiencies than the conventional methods [2].

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2. DROPLET GENERATION IN A MICROFLUIDIC T-JUNCTION

The emulsion production experiments were conducted in rectangular 200µm x 75µm microfluidic T-junction fabricated from transparent polydimethyl siloxane (PDMS) material using soft lithography techniques. Syringe pumps were used to supply fluids into the device. The deionised water was fed on the side arm and the mineral oil (density = 840 kg/m$^{3;}$ viscosity = 0.026 Pa.s) was fed in the main arm, as illustrated in Figure 1. Sorbitan monolaurate (Span20®) surfactant (1% v/v) was dissolved in the oil phase, resulting in the interfacial tension of ~ 0.003 N/m. The flow was imaged with a digital camera capable of capturing up to 1200 frames per second under an optical light microscope using a 10x magnification objective lens.

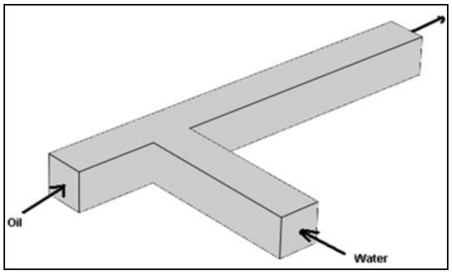

Figure 1: *Illustration of the fluids entry into the microfluidic T-junction.*

The behaviour of microfluidic flows differs from large scale flows, primarily, due to dominance of surface forces such as viscosity and interfacial or surface tension over volume forces such as gravity and inertia. This can be illustrated by the scaling law[1]:

$$\frac{surface\ forces}{volume\ forces} \propto \frac{L^2}{L^3} = L^{-1} \xrightarrow[L\to 0]{} \infty \qquad \text{Eqn. 1}$$

Generation of emulsions in micro-sized channels exploits the balance between these forces. In particular, the balance between the interfacial and the viscous forces is most significant.

The flow patterns (Figure 2) were determined by variation of the volumetric flowrates of both the continuous phase (Q_c) and the dispersed (water) phase (Q_d). The flow pattern map (Figure 3) was constructed from 270 flow patterns. The flow patterns are plotted for Ca_c of the continuous or oil phase for values ranging between 0.011 and 0.38 against the flow ratio, Q_d/Q_c, which is directly proportional to Ca_d and Re_d. At low to intermediate Q_c values, droplets, cobbles and plugs are dominant at Q_d/Q_c values between 0.01 and 1, above which unstable flow begins to prevail. At higher Ca_c values the instabilities can begin occurring in the limit of Q_d/Q_c equal to 1 and below. The long wavelength instabilities begin at the junction and propagate in the main channel.

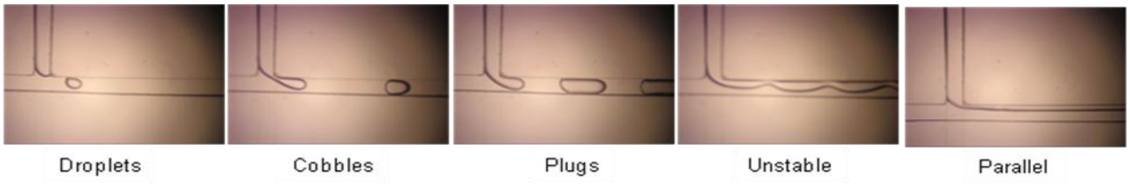

Figure 2: *Various flow patterns in a T-junction microchannel.*

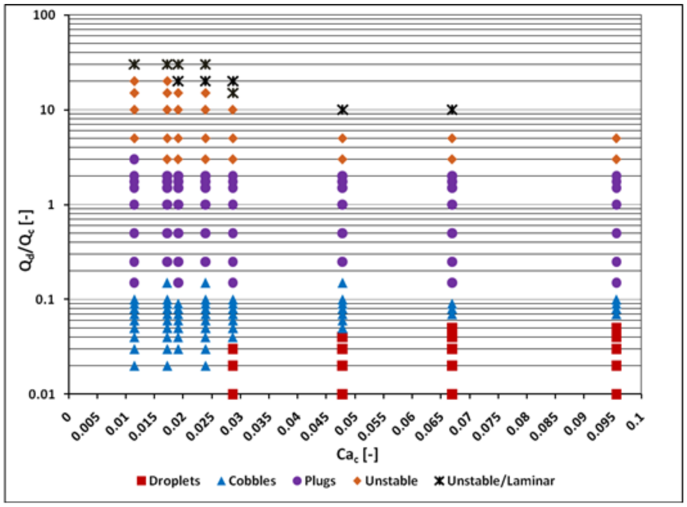

Figure 3: *Variation of flow patterns in a T-junction microchannels as a function the capillary number of the oil phase (Ca_c)*

3. MODELLING AND SIMULATION

The CFD modelling and simulation was achieved using COMSOL Multiphysics software program, whose numerical scheme is based on a finite element method (FEM). The fluid-fluid interface model was based on the conservative level set method (LSM) by Olsson and Kreiss [3]. The fluid-fluid interface was implicitly represented by level set function φ, where $\varphi = 0$ for the oil phase , $\varphi = 1$ for the water phase and $\varphi = 0.5$ at the interface. The Navier-Stokes equations (Eqn. 2-3) and the level set equation (Eqn. 4) were coupled and solved simultaneously.

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t}+\mathbf{u}\cdot\nabla\mathbf{u}\right)-\nabla\cdot\left[\mu\left(\nabla\mathbf{u}+\nabla\mathbf{u}^{T}\right)\right]+\nabla p=\mathbf{F} \qquad \text{Eqn. 2}$$

$$\nabla\cdot\mathbf{u}=0 \qquad \text{Eqn. 3}$$

$$\frac{\partial\varphi}{\partial t}+\mathbf{u}\cdot\nabla\varphi=\gamma\nabla\cdot\left[\varepsilon\nabla\varphi-\varphi(1-\varphi)\cdot\mathbf{n}\right] \qquad \text{Eqn. 4}$$

where $\mathbf{F}=\sigma\kappa\delta\,\mathbf{n}$, $\kappa=\nabla\cdot\mathrm{n}$, $\delta=6\left|\nabla\varphi\right|\left|\varphi(\varphi-1)\right|$, $\mathbf{n}=\frac{\nabla\varphi}{\left|\nabla\varphi\right|}$ and σ is the interfacial tension.

The γ parameter controls the interface thickness and was assumed to be equal to the mesh size. Interface is reinitialised using the ε parameter which was approximated to the maximum velocity of the flow. Density (ρ) and viscosity (μ) were determined from Eqn. 5-6 based on the respective fluids:

$$\rho=\rho_o+\left(\rho_o-\rho_w\right)\varphi \qquad \text{Eqn. 5}$$

$$\mu=\mu_o+\left(\mu_o-\mu_w\right)\varphi \qquad \text{Eqn. 6}$$

The 2D simulations results (Figure 4) showed a similar flow behaviour to the recorded images (Figure 5).Although shape and orientation of the droplets were similar there was variation in droplet size between the two methods. The deviation between the CFD model and experiments was attributed to modelling approach which excluded the variations in contact angle between the two fluids and the channel surface which occur in experimental conditions.

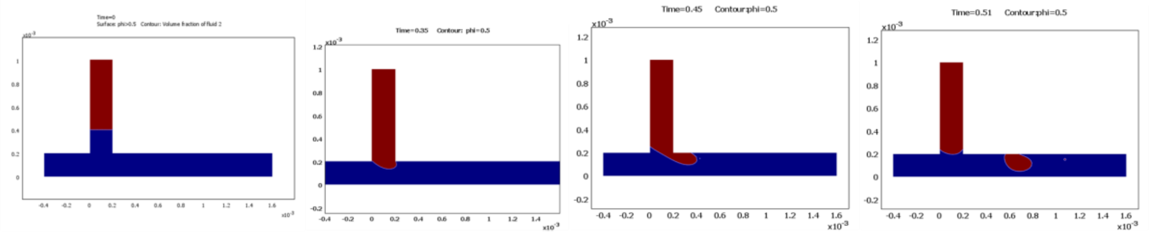

Figure 4: *Snapshots of two-dimensional (2D) simulation sequence of w/o droplet formation in microfluidic T-junction corresponding to the experiment shown in Figure 2.*

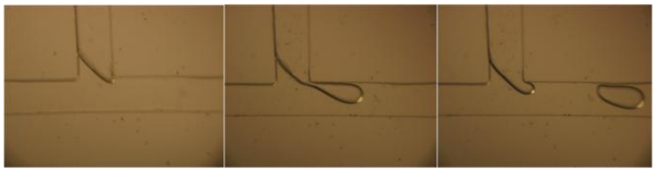

Figure 5: *Snapshots showing sequence of w/o droplet breakup in a 200 µm wide microfluidic T-junction.*

4. CONCLUSIONS

Various two-phase flow regimes exist in a microfluidic T-junction as a function of the capillary number and the relative flows of the two immiscible fluids. Experiments and CFD provide useful tools for further study of biphasic microfluidic flows. However, further experimental validation of CFD results need to be conducted.

ACKNOWLEDGEMENTS

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REFERENCES

[1] Joanicot, M. & Ajdari, A. Droplet control for microfluidics. *Science 309 (2005) 887-888.*

[2] Huebner A, Sharma S, Sria-Art M, Hollfelder F, Edel JB, & deMello AJ. Microdroplets: A sea of applications? *Lab. Chip 8(2008) 1244-1254.*

[3] Olsson, E. & Kreiss, G. A conservative level set method for two phase flow. *J. Comp. Phys. 210, 1(2005) 225-246.*