Effect of phase velocity and surface tension on droplet formation in flow-focusing device

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Abstract

Two-dimensional computational fluid dynamics (CFD) simulation was performed to study droplet formation of liquid-liquid two-phase flow in a flow-focusing device. The VOF technique was used to simulate the two phase interface. Among the effective parameters that govern on droplet formation process, the inlet velocity of two phases and the surface tension are two of the most important parameters in the droplet formation process that has influence on droplet size. The simulation results revealed that as continuous phase velocity increases from 0.001 m/s to 0.018 m/s, the droplet size decreases and as dispersed phase velocity increases from 0.002 m/s to 0.016 m/s, the droplet size increases, but the coalescence of the droplets is occurred. The results also showed that as surface tension increases from 0.0001 N/m to 0.013 N/m the frequency of droplet formation decreases, while the droplet size increases.

Keywords: CFD simulation, Inlet velocity, Surface tension, Flow-focusing device, VOF method

Introduction

Droplet formation of a fluid in a second immiscible fluid has many practical applications in microfluidic such as biological processes, chemical analyses, drug delivery, heat exchangers etc [1]. Nowadays microdevices are commonly used to generate mono-dispersed droplets. A series of simple microfluidic devices have been proposed for droplet generation like T junctions, co-flow devices, flow-focusing devices and microchannel terraces. Among flow-focussing devices micro cross-junctions have received a special attention for the generation of mono-dispersed droplets. In these devices, the continuous flow is introduced by means of two lateral junction branches in order to squeeze and shear off the interface of an immiscible liquid used as the dispersed phase and to introduce it inside the junction through its central microchannel [2]. Computational fluid dynamics (CFD) simulations could be used as an alternative tool to understand the unknown and complicated physics that govern this process [3]. Lashkaripour [3] studied droplet formation process in flow-focusing devices numerically. They showed the flow rate ratio and capillary number are the two primary parameters that affect droplet size, while capillary number showed more dominance in comparison to flow ratio. Yongping [4] investigated the formation of emulsion droplets in a coflowing microchannel using the VOF
method. They studied effect of viscosity ratio, capillary and weber number. Lu peng [5] studied the effect of interfacial tension on the droplet formation in the flow-focusing devices, also, the effect of addition surfactant to the fluid was investigated. Liu [6] studied droplet formation in microfluidic cross-junction by using Lattice Boltzman multiphase model. They investigate the influence of flow rate ratio, capillary number and found the channel geometry plays an important role in droplet breakup process. Gupta [7] studied effect of geometry on droplet formation in the squeezing regime used by Lattice Boltzman model in a microfluidic T-junction. In this study, two-phase flow in droplet formation process within a flow-focusing device has been studied. Then the effect of velocity of the continuous and dispersed phases and the surface tension on the droplet size has been investigated in details and results has been presented.

Numerical simulation
Volume of fluid method
Several methods have been previously used to approximate free boundaries in finite difference numerical simulations. A simple, but powerful, method is described that is based on the concept of a fractional volume of fluid (VOF). This method has been shown to be more flexible and efficient than other methods for treating complicated free boundary configurations. Thus, the VOF method provides a simple and economical way to track free boundaries in two or three-dimensional meshes [8]. In this study the volume of fluid method was used for simulation to track the interface between two immiscible fluids.

Simulation setup
Fig. 1 shown the simulation setup. Our system has three inlets, two inlets for continuous phase and one inlet for dispersed phase. The continuous phase (oil) flows into the main channel from both sides. The dispersed phase (water) enters the microchannel and was broken up to droplets at the cross-junction by the shear effect of the continuous phase. The physical model of the simulation is shown in Fig 1(a). The mesh model was constructed using Workbench 19.2, and the numerical computations were conducted using the Fluent 19.2 (Ansys Inc) software package. In Fig 1(b) mesh information is shown in near the cross-junction.

Physical properties of two phases are shown in Table 1. The boundary conditions are,

1. Velocity inlet for water at channel entrance equal to 0.004 m/s
2. Velocity inlet of oil at side channel entrance equal 0.006 m/s
3. The outlet of main channel was defined as pressure outlet with zero gauge pressure.
4. All channels walls were defined as stationary walls and no slip condition was applied
5. The contact angle of dispersed phase was considered as 140°.

Table. 1. Physical properties of continuous and dispersed phases.

<table>
<thead>
<tr>
<th>The physical parameters</th>
<th>Disperse phase (Water)</th>
<th>Continuous phase (Oil)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dynamic viscosity (kg/m.s)</td>
<td>998</td>
<td>900</td>
</tr>
<tr>
<td>Density (kg/m$^3$)</td>
<td>0.001</td>
<td>0.025</td>
</tr>
<tr>
<td>Interfacial tension (N/m)</td>
<td>$5 \times 10^{-3}$</td>
<td></td>
</tr>
</tbody>
</table>
Model theory

For simulation, the continuity and incompressible Navier-Stokes equations for both dispersed phase and continuous phase are governed,

\[ \frac{\partial \rho}{\partial t} = \nabla \cdot (\rho \mathbf{u}) = 0 \]  \hspace{1cm} (1)

\[ \frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla P + \rho \mathbf{g} + \nabla \cdot [\mu (\nabla \mathbf{u} + \nabla \mathbf{u}^T)] + F_s \]  \hspace{1cm} (2)

\[ \frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \mathbf{u}) = 0 \]  \hspace{1cm} (3)

\( \mathbf{u} \) is the velocity vector field, \( P \) is pressure field and \( \mathbf{g} \) is the gravitational force. The parameter \( \alpha \) is the phase fraction parameter based on VOF method. Parameters \( \rho \) and \( \mu \) are mixed fluid density and viscosity which are based on the weighted average of the distribution of the phase fraction,

\[ \mu = \alpha \mu_c + (1 - \alpha) \mu_D \]  \hspace{1cm} (4)

\[ \rho = \alpha \rho_c + (1 - \alpha) \rho_D \]  \hspace{1cm} (5)

The last term in Eq. (2), \( F_s \), is the surface tension forces that are simulated by CFS as an external force applied to the volume. This force term is defined as,
\[ F_s = \sigma k(\nabla \alpha) \]  

(6)

where in \( \sigma \) is the surface tension between the two phases and \( k \) is the local curvature of the interface \( (k = \nabla \cdot \left( \frac{\nabla \alpha}{|\nabla \alpha|} \right)) \).

**Results and discussion**

**Effect of velocity of continuous phase on droplet size**

First the effect of continuous phase velocity on the droplet formation process was investigated. Fig. 2 shows the results of the simulations. As the continuous phase velocity increases droplet size decreases, meanwhile, dispersed phase velocity was kept constant at 0.004 m/s. As Deng [9] also showed, the increase of continuous phase velocity results in a greater shear force on the dispersed phase that is required to produce smaller droplets. As shown in Fig. 2 production of satellite droplets increased.

![Satellite droplet](image)

**Fig. 2. Velocity of continuous phase: (a)\( v = 0 \cdot 001 \frac{m}{s} \), (b)\( v = 0 \cdot 003 \frac{m}{s} \), (c)\( v = 0 \cdot 006 \frac{m}{s} \), (d)\( v = 0 \cdot 009 \frac{m}{s} \), (e)\( v = 0 \cdot 012 \frac{m}{s} \), (f)\( v = 0 \cdot 015 \frac{m}{s} \) and (g)\( v = 0 \cdot 018 \frac{m}{s} \).**

**Effect of velocity of dispersed phase on droplet size**

When continuous phase velocity is fixed at 0.006 m/s, the increase of the dispersed phase velocity causes increase in droplet size. The distance between the droplets is reduced and with further increase of dispersed phase velocity the droplets are jointed. As shown in Fig. 3 while the dispersed phase velocity increases, the droplet formation regime changes from dripping to wide jetting. This regime is visible with increasing velocity of the dispersed phase fluid.
Effect of surface tension on droplet size

As shown in Fig. 4, increasing the surface tension between fluids causes the droplet formation process to change while other parameters are constant. As Han [10] showed, by an increase in surface tension, it was found that the time required for droplet formation increased and also the frequency of droplet formation decreased. In other words, the droplet break up requires more force and therefore the droplet formation time is increased thus the droplet enlarged. When the surface tension is very low, a long jet of water is formed but the droplet break up process does not occur.

Conclusions

A CFD simulation on the droplet formation of water in oil in a flow-focusing device using the VOF model was presented. The CFD simulations have been carried out for different continuous and dispersed phase velocities. Our simulation results show that with increasing of velocity of continuous phase droplet size decreases. As velocity of dispersed phase increases droplets size
increases. When velocity of dispersed phase increases, two regimes were observed. This is due to the interaction between two immisible fluids and the sizes of produced droplets were different. The next parameter to be investigated was surface tension. The result showed that increasing the surface tension increases the droplet break up time and droplet size. The frequency of droplet formation is also reduced. When the surface tension is greater than 0.0012 N/m no droplet was produced.

References


