Effect of Interfacial Tension on Droplet Generation in T-Junction Microfluidic Device

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Abstract

Droplet generation in microfluidics is a powerful technique to get monodispersed emulsions and droplet size manipulation can be very advantageous in a wide area of applications such as pharmaceuticals, drug delivery, food products, chemical synthesis and biomedical applications. In the present study, the effect of interfacial tension on droplet size and droplet generation frequency is observed using COMSOL Multiphysics® software package version 5.3. To observe the variation in droplet size and generation frequency, interfacial tension is varied from 5 mN/m to 30 mN/m. Experimentally, Interfacial tension can be varied by changing the concentration of the surfactant added to continuous/dispersed phase. As the concentration of the surfactant increases, interfacial tension decreases. The present work is limited only to the numerical investigation of the interfacial tension effect in W/O emulsions with water as dispersed phase and oil as the continuous phase. In this study, laminar two-phase flow level set method is used. Since the droplet generation in T-junction microfluidic device takes place when viscous force by flowing stream of continuous phase overcomes the surface tension force. From scaling analysis, it is found that droplet diameter scales as the reciprocal of the Capillary number. Keeping the other parameters such as the velocity of flowing streams, viscosity, channel width/diameter constant, droplet diameter is expected to increase with the increase in interfacial tension. Similar effects have been studied on Flow focusing device by Lu Peng et al. [4] and on T-junction by Shazia et al. [5]. The results obtained for different interfacial tension are following the expected variation. It is observed that with increasing interfacial tension droplet size is increasing and droplet generation frequency is decreasing. It can be concluded from the study that interfacial tension variation due to surfactant concentration control will consequently manipulate the droplet size.

Keywords: Microfluidics; level set method; computational fluid dynamics; emulsion

1. Introduction

In recent years, research in microfluidics has obtained a considerable progress and it is leading to the possibilities in a wide range of applications such as drug delivery, biomedical applications, chemical synthesis [1-3]. Droplet generation in microfluidics involves the flow of immiscible liquids to form mono-dispersed droplets in a microfluidic channel. Mono dispersed droplet generation finds the applications in food products, pharmaceuticals, etc. Several techniques have been proposed for droplet generation in microfluidics. There are mainly three strategies to make a microfluidic droplet generator, flow focusing, co-flow and cross-flow or T-junction. T-junction microfluidic device involves flow of two immiscible fluids i.e. continuous phase and the dispersed phase in channel at right angle as shown in the figure 1. If we talk about the dynamics of droplet formation, in flow focusing and co-flow devices droplet formation is strongly dependent on the inertia of the fluids interacting. However, in T junction devices, droplet formation is mainly controlled by the shear force and interfacial force. The droplet formation in T junction takes place when shear force acting on the interface between the two fluids overcomes the force due to interfacial tension.

Many researchers have experimentally as well as numerically studied different parameters affecting the droplet formation. Parameters such as viscosity ratio [6] of the continuous and dispersed medium, flow rates of the fluids [7], geometry of the channel, interfacial tension, injection angle [8], wettability of the liquid affects the droplet formation. To study the effect of interfacial tension, many experimental studies have been performed for T junction microfluidic device by adding surfactant at different concentration and hence controlling the droplet diameter. Lu Peng et al. [4] studied effect of adding surfactant Tween 20 in a flow focusing device and observed experimentally and also through simulation the variation of droplet diameter and generation frequency. Shazia et al. [5] did the similar experiment on T junction device using Span80 surfactant. In present study, focus is on studying numerically the effect of interfacial tension on the droplet diameter and droplet generation frequency for water in oil monodispersed emulsion. For the formation of W/O emulsions, hydrophobic channels are used so for present simulations all the channel are considered as a wetted wall with water contact angle of 135 degrees. However Li et al. [2] reported that both W/O as well as O/W emulsions can be obtained in a single microfluidic device using surfactants at required concentrations. In further section, scaling analysis has been done to show how the interfacial tension is related to the droplet diameter based upon a non-dimensional number called Capillary number. Capillary number is defined as the ratio of shear force to the interfacial force. In T junction devices, there are mainly three different regimes depending upon the physical parameters such as flow rates, viscosities, geometry and interfacial tension. In other words, one can say that regimes exist as per the Capillary number. The three regimes are found to be squeezing, dripping and jetting regime. Squeezing regime occurs at low Capillary number and formation of larger droplet takes place since the interfacial tension is dominating and detachment takes place due to the upstream pressure when droplet formed almost blocks the channel. It is found that the effect of interfacial tension on droplet diameter in squeezing regime is not significant and droplet size is mainly manipulated by the flow rates. In dripping regime, capillary number is higher and droplet formed doesn’t block the microchannel. Droplet diameter and Capillary number can be conveniently defined in this case based upon the scaling analysis. Jetting regime occurs at very high capillary number, long neck is formed and very small droplets are formed.

In this paper, interfacial tension is varied from 5 mN/m to 50 mN/m. Dispersed phase and continuous phase velocities are 50 mm/sec and 100 mm/sec respectively.

2. Numerical Simulation:

To simulate the problem, in COMSOL Multiphysics laminar two phase incompressible flow is considered and level set method is used for interface tracking.

Problem Formulation

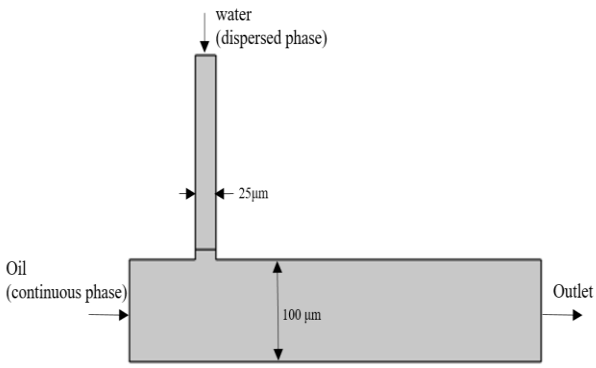


Figure 1: 2D Geometry of the T junction microchannel

In the problem schematic shown in figure 1, microchannel channel diameter is taken as 100 μm and the diameter of the cross channel through which dispersed phase is entering has been taken as 25 μm. The physical properties such as density and viscosity of water and oil are user defined values as shown below in the Table 1.

Phase	Inlet Velocity (mm/s)	Density (kg/m^3)	Viscosity (Pa s)
Water	50	1000	0.001
Oil	100	900	0.02

Table 1: Properties of fluids used

Governing Equations

The fluid flow is considered as incompressible and laminar and density and viscosity of the liquids are constant throughout the flow. The governing equation that defines the fluid flow are the Navier Stokes equations for mass conservation and momentum conservation. The equations for a pair of immiscible liquids can be written as:

$$\nabla\, u_i = 0 \quad (1)$$

$$\rho\left(\frac{\partial u_i}{\partial t} + u_i \cdot \nabla\, u_i\right) = -\nabla p_i + \nabla\, \tau_i + F_s + \rho g \quad (2)$$

where subscript i represents the fluid, ρ is the fluid density, u is the velocity vector, μ is the fluid dynamic viscosity, t is time p is fluid pressure, g is the acceleration due to gravity, F_s is the surface tension force.

The interface between the water droplet and oil phase are tracked using the Level Set method. The Level Set method is an Eulerian approach to track the interface for multiphase flow problems [9]. Level set method is the most favourable method track the moving interfaces. The level set method uses a function called level set function (ϕ). The level set function changes its value smoothly across the interface from 0 to 1 where ϕ=0 is water and ϕ=1 is oil medium and ϕ=0.5 represents the interface contour.

The equation representing the convection of reinitialized level set function is given as:

$$\rho\left(\frac{\partial \phi}{\partial t} + \nabla(\phi u)\right) = \gamma\left[\epsilon\nabla \cdot \nabla\phi - \nabla \cdot \left(\phi(1-\phi)\frac{\nabla\phi}{|\nabla\phi|}\right)\right]$$

The above equation is coupled to Navier Stokes equation for continuity and momentum conservation to get the advection for level set function. The level set function smoothens the density and viscosity jumps across the interface.
The surface tension force is calculated by the following expression:

$$F_s = \nabla \cdot [\sigma(I - nn')\delta]$$

Where I is the identity matrix, σ is the surface tension, and δ is the Dirac delta function, n is the interface
Normal which is written as

$$n = \frac{\nabla\phi}{|\nabla\phi|}$$

and delta function is given by following equation

$$\delta = 6|\phi(1-\phi)||\nabla\phi|$$

Boundary Conditions

At two respective inlets of oil and water, normal flow velocity is specified as given in Table 1. Outlet is given as zero gauge pressure. Physics controlled fine meshing has been done on the two dimensional geometry. Total number of triangular elements created is around 3000. The walls are selected as wetted wall with water contact angle of 135 degrees.

3. Scaling Analysis

As droplet formation in T-junction microfluidic device is a complicated mechanism involving different forces such as interfacial tension, viscous shear, pressure drop. As discussed in the introduction the role of upstream pressure is significant in squeezing regime. To develop a relation between interfacial tension/Capillary number and droplet size, scaling analysis can be useful.
As viscous shear force competes with the interfacial tension force, therefore,

Interfacial tension force ~ Viscous Drag

$$\sigma d_d \sim \mu_c U_c D_{drop}$$

$$D_{drop} \sim \frac{\sigma\, d_d}{\mu_c U_c}$$

Capillary number for continuous phase can be written as,

$$\mathrm{Ca} = \frac{\mu_c U_c}{\sigma}$$

Therefore,

$$D_{drop} \propto \frac{1}{\mathrm{Ca}}$$

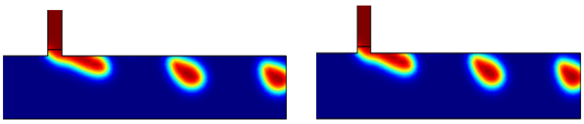
and

$$D_{drop} \propto \sigma$$

where, D_{drop} is the diameter of the droplet formed, σ is interfacial tension, μ_c is dynamic viscosity of continuous medium, U_c is flow velocity of continuous medium, d_d is diameter of dispersed medium.

4. Results and Discussions

It has been observed that at very low value of interfacial tension, size of droplet formed is very small. Due to very low value of interfacial, right after the formation of droplet shape is not spherical. At low value of σ, jetting regime is existing as shown in the figure 2. There is negligible change in the droplet size at σ=5mN/m and σ=10mN/m.



(a) (b)

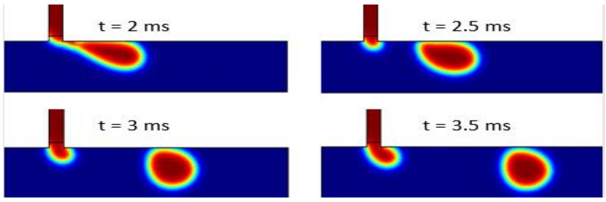
Figure 2: Droplet generation at 5mN/m (a) and 10mN/m (b) at time t=4 ms

All the simulations have been performed for 20 time steps ranging from 0.5 ms to 10 ms.

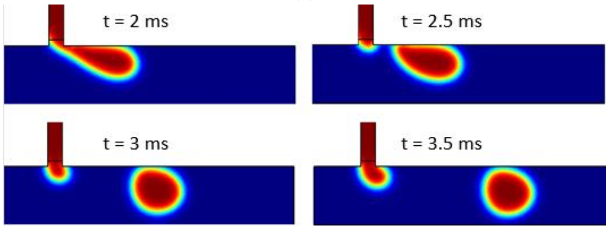
As the value of σ is increased to 15 mN/m and beyond there is appreciable increment in the droplet size as shown in the following figures. It can be seen that droplet formation is somewhat different unlike the previous jetting case, here dripping regime is starting to exist.

Figure 3: Droplet formation at σ = 15 mN/m at t=4 ms**.**

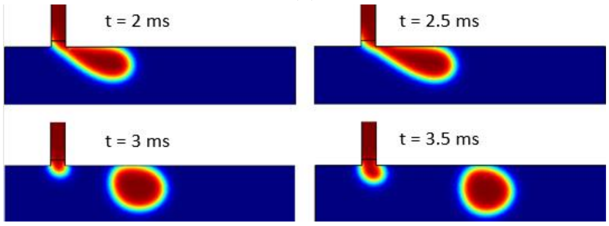
The following figures represent the detailed droplet formation process at σ values from 20 mN/m to 50 mN/m.



(a)



(b)



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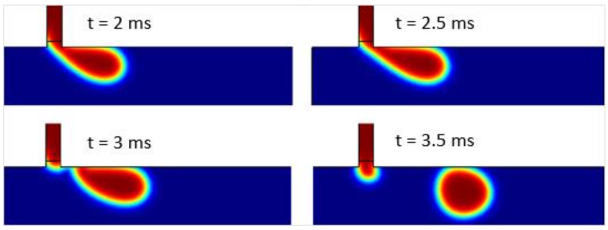

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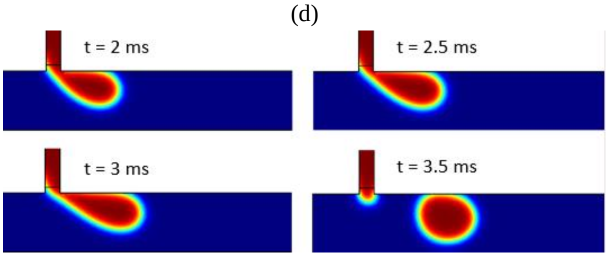

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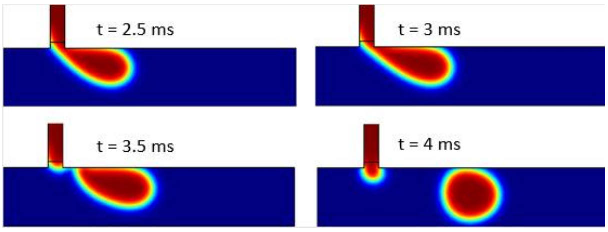
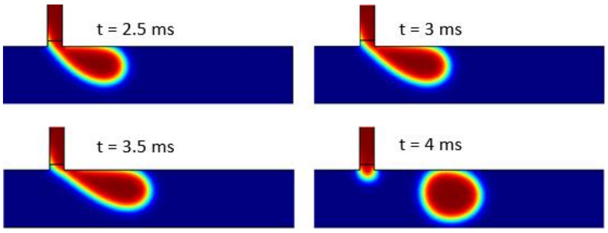


(f)



(g)

Figure 4: Droplet formation for σ ranging from 20 mN/m (a) to 50mN/m (g) with steps of 5 units.

It is clear from the simulation results that the droplet size is increasing as the interfacial tension is increased. Droplet diameter and generation frequency have been evaluated through some image processing and plots have been made as shown in Figure 5.

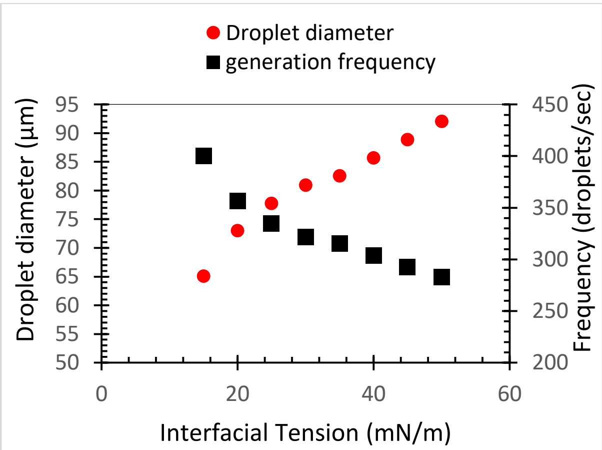


Figure 5: Variation of droplet diameter and generation frequency with interfacial tension

5. Conclusions

In this study, it is shown how interfacial tension is affecting the size of the droplet generated. It is clearly observed that the droplet size is increasing as σ is increased because of increased interfacial tension force keeping the other things constant. However, the effect is negligible when σ is very low i.e. very high Ca.

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