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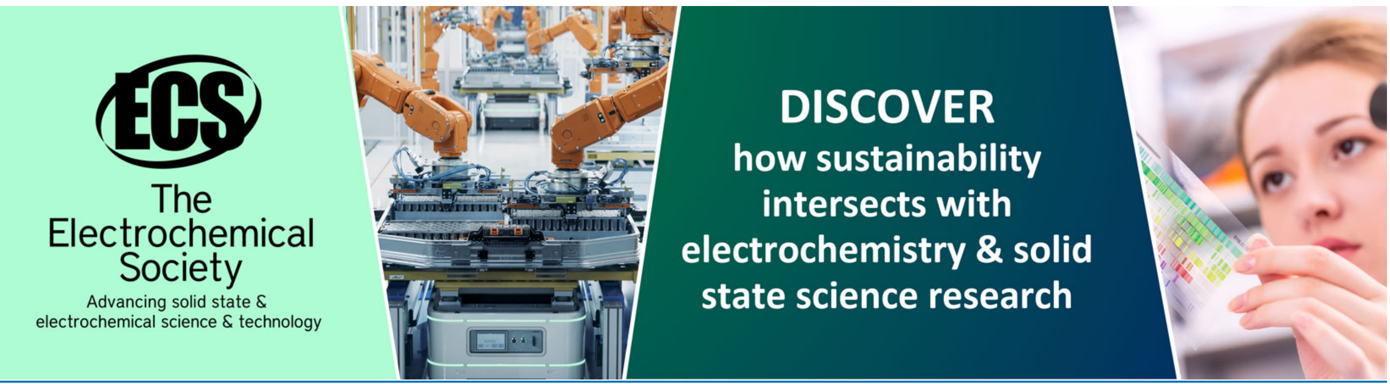

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3D simulation of droplet coalescence in T-shaped microchannel

Lixiang Li, Ziheng Lin and Wenyuan Fan*

School of Chemistry and Chemical Engineering, Tianjin University of Technology, Tianjin, China

*Corresponding author e-mail: fwy924@163.com

Abstract. Three Droplet coalescence behaviour in T-shaped microchannel under different conditions is investigated numerically using coupled volume of fluid and level set (CLSVOF) method. The effects of continuous phase (water) flow rate and physical properties of dispersed phase are examined respectively. The results show that with the increase of water flow rate, the volume of coalesced droplet decreases, its deformation increases but coalesced time hasn't changed significantly. Droplet coalescence time go down, however the aspect ratio of the coalesced droplet increase first and then decrease in the order of pentanol, octanol and decanol, with no obvious impact on coalesced droplet volume.

1. Introduction

As an important branch of microfluidics, Droplet microfluidics [1] can precisely manipulate the behavior of microdroplet, in which droplet coalescence plays a particularly important role in chemical synthesis, preparation of micro-nano particles [2]. T-type microchannel is more widely used due to their simple structure and precise control of droplet size compared with other various types of microfluidic devices. Microdroplet coalescence behavior has been paid attention by more researchers owing to its wide application in such fields as chemistry, biology and soon. Fidalgo et al. [3] coalesced various sizes of micro droplets in different numbers by using controlled PDMS microvalves. Liu et al. [4] studied droplet coalescence by changing the wettability of the wall. Link et al. [5] focused the droplet coalescence under outer field such as an electric field, a magnetic field and a laser. Deng et al. [6] achieved controllable one-to-one coalescence of surfactant-stabilized nanoliter water drops by surrounding one of the drops with a thin layer of immiscible wetting fluid. Recently, Deng et al. [7] performed the drop-coalescence-triggered microreaction in microchannels for pH indicator and syntheses of functional materials including micro and nanoparticles.

On the other hand, numerical simulation method has become an increasingly popular approach due to its high capability to obtain some essential physical information. Among several methods, volume of fluid [8] and level set method [9] were often adopted to consider the coalescence and breakup behaviour of bubbles or droplets because of their high interface capturing accuracy. In this paper, a coupled level-set/volume-of-fluid (CLSVOF) method has been employed to explore bubble coalescence regime, and reveal the effects of continuous phase flow rate and physical properties of dispersed phase on droplet coalescence in T-type microchannel.

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2. Simulation

2.1. CLSVOF Model

The continuity and momentum equations for two isothermal, incompressible, immiscible fluids can be written as:

$$\nabla \cdot \boldsymbol{U} = 0 \tag{1}$$

$$\rho(H)\left(\frac{\partial(\boldsymbol{U})}{\partial t} + (\boldsymbol{U}\cdot\nabla)\boldsymbol{U}\right) = -\nabla P + \nabla\cdot\left[2\mu(H)\left(\nabla\boldsymbol{U} + \nabla^T\boldsymbol{U}\right)\right] + \rho(H)\boldsymbol{g} + \boldsymbol{F}_s \tag{2}$$

Where $\boldsymbol{U}$ is the velocity vector, P the pressure, $\boldsymbol{g}$ the gravitational acceleration, $\boldsymbol{F}_s$ a body force due to surface tension, $\rho(H)$ and $\mu(H)$ are the density and dynamics viscosity.

$$\rho = \rho_l H + (1-H)\rho_g \tag{3}$$

$$\mu = \mu_l H + (1-H)\mu_g \tag{4}$$

Where ρ_l and ρ_g are the density of the liquid and gas, μ_l and μ_g are the viscosity of the liquid and gas, respectively. The continuous surface force (CSF) is used to calculate the gas-liquid interface motion, by introducing a body force $\boldsymbol{F}_s$ as following:

$$\boldsymbol{F}_s = \sigma\kappa(\phi)\nabla H(\phi) \tag{5}$$

Where σ is the surface tension, and $\kappa(\phi)$ is the local surface curvature. H is a Heaviside function given by

$$H(\phi) = \begin{cases} 1 & if \quad \phi > 0 \\ \frac{1}{2} & if \quad \phi = 0 \\ 0 & if \quad \phi < 0 \end{cases} \tag{6}$$

The level-set function ϕ is introduced and defined as the signed closest distance towards the interface. The local surface curvature, κ, is calculated as follows:

$$\kappa = -\nabla\cdot\frac{\nabla\phi}{|\nabla\phi|} \tag{7}$$

In CLSVOF method, the solution is integrated to both the equations representing the VOF function F and the LS function $H(\phi)$:

$$\frac{\partial F}{\partial t} + \boldsymbol{U}\cdot\nabla F = 0 \tag{8}$$

$$\frac{\partial \phi}{\partial t} + \boldsymbol{U}\cdot\nabla\phi = 0 \tag{9}$$

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2.2. Physical Model
The physical model of the simulation is simplified to a 3D computational domain, two crosses microchannel with their throats were adopted to generate droplets for later coalescence, as shown in Fig. 1. The 0.1 mm mesh with uniform structured grid is chosen based on the analysis effect of the grid size.

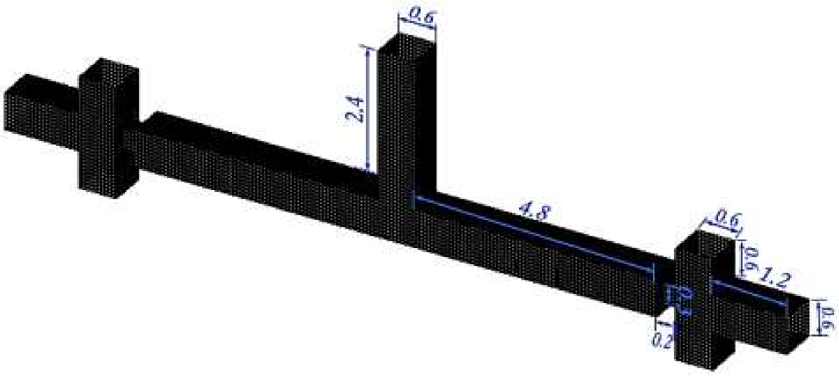

Figure 1. Schematic diagram of solution domain.

3. Results and Discussion

3.1. Coalescence Process and Regime
In the paper, water and three alcohols, including pentanol, octanol, decanol, were employed respectively as continuous phase and dispersed phases. Figure 2 presents the coalescence process of two droplets with the water flow rate of 3.2mm/s and pentanol flowrate of 1.6 mm/s. It can be drawn that the whole droplet coalescence can be divided into 3 stages. In the first stage, two droplets begin to contact with two small tails opposite each other and then merge together; In the second stage, the merged droplet is squeezed gradually with an increasing deformation of its middle part; In the third stage, the deformed droplet recovers a spherical shape with a slightly extrusion in outflow channel.

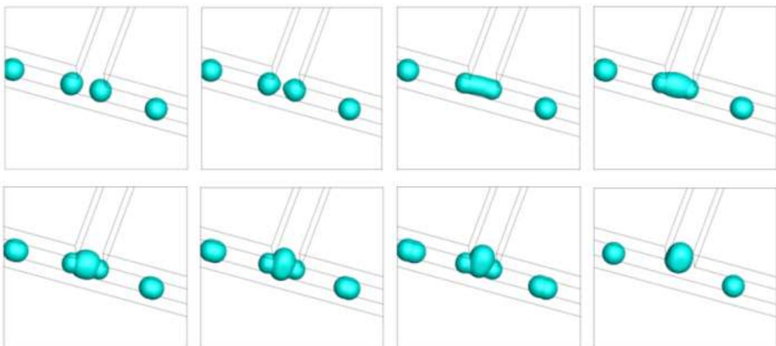

Figure 2. Droplet coalescence process (Δt=0.002ms).

3.2. Effect of Water Flowrate
The effect of continuous phase flowrate on droplet coalescence is shown in Fig.3. It is obvious that the coalescence process follows abovementioned regime for each flowrate. However, while the water flowrate goes up, the volumes of the droplet before and after the coalescing deduce generally. At the same time, the aspect ratio (H/W), as a important parameter for describing droplet defamation, grows from 1.25 to 1.84. The reason can be attributed to the increasing shear effect due to high flowrate of water. However, it is worth mentioning that there is not obvious change in coalescence time.

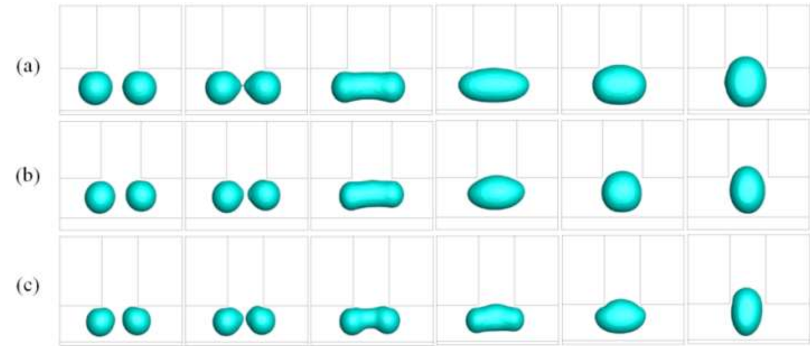

Figure 3. Droplet coalescence for different water flowrate 2.33mm/s (b) 3.20mm/s (c) 4.67mm/s.

3.3. Effect of Three Alcohols

The effect of three alcohols on the droplet coalescence has been compared under water flow rate of 3.2mm/s and alcohol flowrate of 1.6 mm/s, as shown in Fig. 4. It can be seen that for three dispersed phases, two droplets always approach with apparent deformation of two interfaces facing each other, and then collide each other. At the same time, bridge connecting them is formed promptly and the connected droplet start to deform quickly. Finally, droplet's interface is fully recovered to a spherical shape owing to the interfacial tension between two phases. However, the detailed coalescence characteristics under three alcohols conditions are slight differences. In the order of pentanol, octanol and decanol, the whole coalescence time decreases a little, but the aspect ratio of the droplet after coalescence increase first and then decrease. Moreover, the volume of coalesced droplet is not significantly affected by the kind of water-alcohol system.

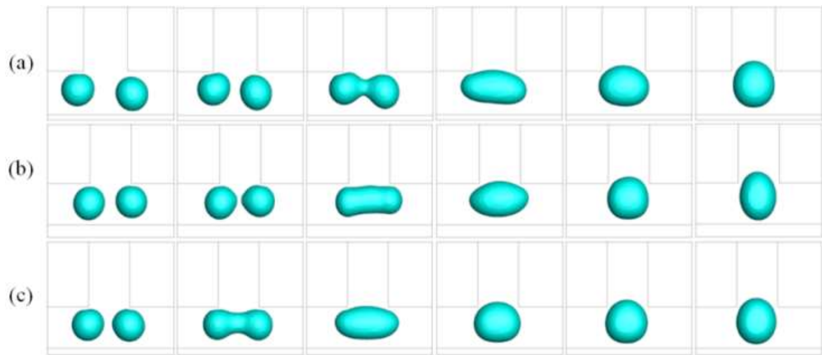

Figure 4. Droplets coalescence for different alcohols (a) pentanol; (b) octanol; (c) decanol.

4. Conclusion

A improved numerical method combined volume of fluid and level set, is applied to study droplet coalescence in T-shaped microchannel. The coalescence regime and the influences of continuous phase and dispersed phase on coalescence characteristics are considered respectively. The following conclusions are drawn.

The whole droplet coalescence can be divided into contact-mergence, squeezing-deformation and recovery three stages.

With the increase of water flowrate, the volumes of the droplet before and after the coalescing deduce generally. But the aspect ratio goes up.

The coalescence time decreases gradually, but the aspect ratio of the after-coalescence droplet increases first and then decrease in the order of pentanol, octanol and decanol.

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