Lattice Boltzmann simulation of droplet formation in T-junction and flow focusing devices

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Droplet formation in T-junction microchannel and flow focusing configuration is numerically studied by using the lattice Boltzmann method. Various parameters including flow rate ratio, capillary number, geometry, and wetting property are investigated. The results show that due to the confinement of the main channel, the T-junction microchannel is prone to generate elliptic droplets, while the flow focusing configuration is likely to generate spherical droplets. In particular, the work shows that the geometry effect, i.e., the width ratio of main channel to lateral channel of T-junction, and the width of the orifice in flow focusing configuration, plays a significant role in the determination of shape and length or the diameter of droplets. It also demonstrates that the lattice Boltzmann method with free energy model is an effective way to simulate the generation of droplets in T-junction microchannel as well as in flow focusing configuration.

1. Introduction

In recent years, emulsions generated by microfluidic devices play critical roles in consumer products, cosmetics, pharmaceuticals for drug delivery, and chemical industries. The size and flow pattern of the droplet are important factors for any emulsion. Particularly, highly monodisperse droplets have been generated via a number of methods in microfluidic devices [1–4]. Thereinto, T-junction microchannels [5–7] and flow focusing configurations [8–10] are two typical devices that depend upon channel geometry to control the generation of droplets.

Studies of droplet generation in microfluidic devices have been performed [11–16]. Several research groups have experimentally investigated various aspects of the droplet generation. Thorsen et al. [17] firstly considered the droplet formation within a T-junction microchannel, and they found that the length of droplet decreases with the increasing of the continuous phase flow rate. Xu et al. [18] discussed the correlations of the capillary number for the continuous phase with the droplet formation in squeezing, transient, and dripping regimes, respectively. Garstecki et al. [19] established a simple scaling law for the length of the droplet that is independent of the capillary number and merely related with the flow rate ratio of the two immiscible fluids. Sivasamy et al. [6] found that the pressure profiles of the dispersed phase and the continuous phase in the squeezing regime change as the droplet breakup process proceeds. Anna et al. [3] designed a flow focusing configuration and studied generation of water droplets by two oil streams forcing a water stream through a narrow orifice. Yobas et al. [10] demonstrated a high-performance flow-focusing geometry with a cusp-like edge orifice for spontaneous generation of monodispersed droplets. Moreover, some other groups have observed that the size of droplets is controlled by the fluid thermophysical properties of the two phases and the flow rates of the two phases [20–23].

Although various studies on the generation of droplets in T-junction and flow focusing devices have been carried out, a fundamental understanding of the flow physics that account for the effect of the geometry of the devices is still missing. In addition, simulation of two immiscible phases flow in complex geometries is a challenging work. Recently, the lattice Boltzmann method has been proved to be a powerful method to simulate complex flows, including microscale porous flow [24], microscale non-Newtonian flow [25], compressible flow [26], and especially two immiscible phases flow in complex geometries [27]. There are several popular multiphase models in the lattice Boltzmann method including the color model [28], Shan–Chen model [29], interparticle potential model [30] and mean-field model [31]. The color model and Shan–Chen model are widely used because of their easy implementation. However, the disadvantages for the color model and Shan–Chen model are that the spurious velocities are high at the interface and the local momentum is not conserved. Meanwhile, the spurious velocities are high at the interface for interparticle potential model and the computing time is quite long for mean-field model. Considering both the strengthness and weakness of each model, the present simulation is based on the free...
energy model of lattice Boltzmann method developed by Swift et al. [32] and later by Liu and Zhang [33], which is of advantages including local momentum conservation, low spurious velocities, relatively thin interface, and gradual diffusion for interfaces of two immiscible phases.

The goal of the present study is to quantitatively and qualitatively investigate various fluids’ properties and flow parameters that affect the generation of the droplets in both T-junction and flow focusing devices. Especially, we focus on the geometry effect, i.e., the width ratio of lateral channel to the main channel of T-junction, and the width of the orifice in the flow focusing configuration, which were usually ignored in earlier investigations. In addition, to the best of the authors’ knowledge, the free energy model of lattice Boltzmann method has not yet been applied to investigate the droplet generation in flow focusing configuration.

2. The model

The present simulations are based on the lattice Boltzmann scheme developed by Swift et al. [32]. A suitable free-energy function is described in this scheme to control the equilibrium properties of the binary system.

2.1. Free-energy model

Following Li et al. [34], the Ginzburg–Landau free energy function is used in the present study

\[ F = \int dr \left[ \rho c_s^2 \ln \rho + \frac{a}{2} \phi^2 + \frac{b}{4} \phi^4 + \frac{\kappa}{2} (\nabla \phi)^2 \right] \tag{1} \]

where \( \rho \) is the total density and \( \phi \) is the order parameter that describes the normalized difference in density of the two fluids. The gradient term relates to the surface tension, and the value of \( \kappa \) is related to the interfacial properties of the interface between two immiscible phases. The parameters \( b \) and \( \kappa \) are always positive, while the parameter \( a \) is always negative. When \( a \) is negative, the phase separation occurs; when \( a \) is positive, there is no phase separation [35]. Two pure phases with \( \phi = \pm \sqrt{-a/b} \) coexist, we set \( a = -b \) so that the equilibrium values for the order parameter are \( \phi_0 = \pm 1 \).

The chemical potential \( \mu \) is given by

\[ \mu = \frac{\delta F}{\delta \phi} = a \phi + b \phi^3 - \kappa \nabla^2 \phi. \tag{2} \]

The dimensionless interfacial tension is given by

\[ \sigma = \frac{4K\phi_0^3}{3\xi^2}. \tag{3} \]

The thickness of interface is defined as

\[ \xi = \sqrt{\frac{2K}{-a}}. \tag{4} \]

In the numerical solution, the interfacial thickness parameter \( \xi \) is a free parameter. \( \xi \) should be set small to keep a sharp interface. However, \( \xi \) cannot be set too small in order to prevent numerical accuracy and instability from occurring at the interface. In our study, we compromise to have \( \xi \approx 3 \) lattice grids.

Considering the unequal viscosities of the two phases, we use the following harmonic averaged viscosity as the mixture viscosity [14]

\[ \frac{v_0}{\nu(\phi)} = \frac{\phi_0 - \phi}{2v_1} + \frac{\phi + \phi_0}{2v_2} \tag{5} \]

where \( v_1 \) and \( v_2 \) are the kinematic viscosity of two phases, respectively. The local relaxation time can be calculated from the dimensionless viscosity \( \nu(\phi) \) by

\[ \tau(\phi) = \frac{v(\phi)}{c_s^2} \frac{1}{2}, \tag{6} \]

where \( c_s \) is the speed of sound.

2.2. Lattice Boltzmann scheme

Based on the work by Liu and Zhang [33], two distribution functions \( f_i(x,t) \) and \( g_i(x,t) \) are used to model the total density \( \rho \) and the order parameter \( \phi \) at each lattice site \( x \) and time \( t \). The evolutions of both distribution functions are governed by the single relaxation time Boltzmann equations of BGK type

\[ f_i(x + e_i\Delta t, t + \Delta t) - f_i(x, t) = -\frac{1}{\tau(\phi)} [f_i(x, t) - f_i^{eq}(x, t)] + F_i(x, t), \tag{7} \]

where \( f_i^{eq}(x, t) \) and \( g_i^{eq}(x, t) \) are local equilibrium distributions defined as [33]

\[ f_i^{eq}(x, t) = \omega_i \left( A_i + \rho \left( \frac{\mathbf{e}_i \cdot \mathbf{u} + (\mathbf{e}_i \cdot \mathbf{u})^2}{c_s^2} - \frac{\mathbf{u}^2}{2c_s^2} \right) \right), \tag{9} \]

\[ g_i^{eq}(x, t) = \omega_i \left( B_i + \rho \left( \frac{\mathbf{e}_i \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{e}_i \cdot \mathbf{u})^2}{2c_s^2} - \frac{\mathbf{u}^2}{2c_s^2} \right) \right). \tag{10} \]

The distribution functions are related to the total density \( \rho \), fluid momentum \( \rho \mathbf{u} \) and density difference \( \phi \) by

\[ \rho = \sum_{i=0}^{8} f_i, \quad \rho \mathbf{u} = \sum_{i=0}^{8} f_i \mathbf{e}_i + \frac{\rho \nabla \phi \Delta t}{2}, \quad \phi = \sum_{i=0}^{8} g_i. \tag{13} \]

In order to obtain the continuum equations pertinent to a binary fluid mixture, the higher-order moments of the local equilibrium distribution functions are defined as [36]

\[ \sum_{i=0}^{8} f_i^{m} e_{ix} e_{iy} = \rho \delta_{x\beta} + \rho u_x u_y, \tag{14} \]

\[ \sum_{i=0}^{8} g_i^{m} e_{ix} = \phi u_x, \tag{15} \]

\[ \sum_{i=0}^{8} g_i^{m} e_{ix} e_{iy} = \Gamma \mu \delta_{x\beta} + \phi u_x u_y, \tag{16} \]

where the subscripts \( x \) and \( y \) represent the components along \( x \) and \( y \) directions, respectively. \( p \) is the pressure, \( \delta_{x\beta} \) is the Kronecker delta, and \( \Gamma = \frac{M}{\rho c_s^4} \) is a coefficient relating to the Cahn–Hilliard mobility \( M = \frac{u_i W_i}{\omega_i} \), where \( u_i \) and \( W_i \) are inlet velocity and inlet width of the continuous phase, respectively, and \( \rho \) is the Peclet number.
For a finite interfacial thickness, straining flows can thin or thicken the interface, which must be resisted by diffusion. Meanwhile, large diffusion would damp the flow seriously. Therefore, an appropriate Peclet number is important to balance the effects of convection and diffusion at the interface. 

2.3. Wetting boundary conditions

Wetting properties are usually characterized by the contact angle on a surface. Young’s law provides the relation between interfacial tensions and contact angle. For a water droplet on a surface, surrounded by oil, the equilibrium contact angle is [37]

$$\cos(\theta) = \frac{\sigma_{\text{oil-water}} - \sigma_{\text{water-wall}}}{\sigma_{\text{oil-water}}},$$  \hspace{2cm} (17)

where $\sigma_{\text{oil-wall}}$ is the interfacial tension of oil with the wall surface, $\sigma_{\text{water-wall}}$ is the interfacial tension of water with the wall surface, and $\sigma_{\text{oil-water}}$ is the interfacial tension of the oil with water interface. The interfacial tension $\sigma_{\text{oil-water}}$ for the oil–water interface is calculated from

$$\sigma_{\text{oil-water}} = \int_{-\infty}^{+\infty} \delta \phi \, dx.$$  \hspace{2cm} (18)

The oil-wall interfacial tension and the water-wall interfacial tension can be calculated as

$$\sigma_{\text{oil-wall}} = \int_{-\infty}^{+\infty} \delta \phi \, dx,$$  \hspace{2cm} (19)

$$\sigma_{\text{water-wall}} = \int_{-\infty}^{+\infty} \delta \phi \, dx,$$  \hspace{2cm} (20)

with $\phi_{\text{wall}} = \phi_0 \tanh (x_{\text{wall}} / \zeta)$ [14], we obtain

$$\sigma_{\text{oil-wall}} = \frac{\kappa \phi_0^2}{\zeta} \left( \frac{2}{3} \left( \phi_{\text{wall}} - \frac{1}{3} \left( \phi_{\text{wall}} \right)^3 \right) \right),$$  \hspace{2cm} (21)

$$\sigma_{\text{water-wall}} = \frac{\kappa \phi_0^2}{\zeta} \left( \frac{2}{3} \left( \phi_{\text{wall}} - \frac{1}{3} \left( \phi_{\text{wall}} \right)^3 \right) \right).$$  \hspace{2cm} (22)

Substituting the values of interfacial tensions into Eq. (15), the contact angle becomes

$$\cos(\theta) = \frac{3}{2} \frac{\phi_{\text{wall}}}{\phi_0} \left( 1 - \frac{1}{3} \left( \frac{\phi_{\text{wall}}}{\phi_0} \right)^2 \right).$$  \hspace{2cm} (23)

3. Model validation

3.1. Static contact angle on partial wetting solid surface

Water droplet on partial wetting surface at different static contact angles $\theta = 45^\circ, 90^\circ$ and $135^\circ$ is simulated. The computational grid is $160 \times 80$ lattice units, and the semi-circular water droplet with the radius $R = 20$ is initially deposited on the solid bottom surface. Each lattice spacing corresponds to $5 \mu m$ in the physical unit. For numerical convenience, the densities of the droplet and matrix are assumed to be unity, and the dynamic viscosity ratio is set to $\eta_d/\eta_t = 1$ [14], where the subscripts $d$ and $c$ denote the dispersed and continuous phases, respectively. The corresponding physical values of density and viscosity are $\rho_d = \rho_c = 1000 \text{ kg/m}^3$ and $\eta_d = \eta_t = 10^{-3} \text{ Pa s}$, respectively. The half-way bounce-back conditions are used for the four boundaries. Fig. 1 shows the converged contours of droplet, where the water droplet (red color) is surrounded by oil (blue color). Fig. 2 shows the contact angles measured from the converged contours compared with the theoretical solution. The result is in linear relationship between the order parameter and the contact angle, and the numerical results are in good agreement with the analytical solution of

$$\cos(\theta) = \frac{1}{2} \frac{\Delta \eta_t}{\eta_c} \left( 1 - \frac{1}{3} \left( \frac{\Delta \eta_t}{\eta_c} \right)^2 \right)$$  \hspace{2cm} [14].

3.2. Taylor deformation under shear flow

Taylor deformation is often employed to investigate droplet deformation behavior in a binary model. A droplet is placed between two shearing plates which are moving at the opposite directions to obtain a linear shear in the Stokes regime. The droplet deformation is a function of the shear rate $\gamma$, where $\gamma = u_p/h$ with $u_p$ being the velocity of the moving plate, and $h$ being the height of the channel. Three dimensionless parameters, i.e., capillary number, Reynolds number and Peclet number are given by $Ca = \gamma R$, $Re = \frac{u_p R}{\nu}$, and $Pe = \frac{u_p R}{\nu} = \frac{h}{\zeta}$ [14], where $R$ is the droplet radius, $\nu$ is the density of droplet, and $\eta$ is the dynamic viscosity of matrix fluid. The densities of the droplet and matrix are assumed to be unity as before, $\zeta$ is the thickness of the interface, $a$ is a parameter in Eq. (1), and $M$ is the mobility. The relaxation parameter $\tau$ in the lattice Boltzmann method is related to $M$. Generally, we have $\tau = \frac{M}{R} + \frac{1}{2}$ and usually set $\tau = \frac{1}{2}$ to minimize numerical errors of the convection–diffusion scheme [38]. In the simulation, we set $Pe = 3, \eta_d/\eta_t = 1$, and $R = 10$. Finally, the droplet reaches a steady state of an elliptic shape, and the ellipse is usually characterized by the deformation parameter [39]

$$\text{Deformation} = \frac{L - B}{L + B}.$$  \hspace{2cm} (24)

where $L$ and $B$ are the half-length and half-width of droplet, respectively. For a droplet in the Stokes regime with small capillary number, the deformation follows a theoretical relation as [40].

$$\text{Deformation} = f \left( \eta_d/\eta_t \right) \text{Ca}.$$  \hspace{2cm} (25)

Fig. 3 presents the stable interface profiles of deformed droplet at six different capillary numbers for $\eta_d/\eta_t = 1$, which is depicted by the contour line of $\phi = 0$, and we find that all profiles cross two fixed points. With the increasing capillary number, the deformation of the droplet becomes more serious. The interface profiles are in good agreement with the numerical results of boundary integral method in [41].

Fig. 4 shows the deformation as function of the capillary number. The linear relationship of $\text{Deformation} = 1.484 \text{Ca}$ between the deformation and capillary number is obtained based on the present simulation results.

With the growing of the capillary number, the droplet breaks up when the capillary number exceeds a critical value. As shown in Fig. 5, the droplet breaks up in a shear field at $Ca = 1.0$. The present profiles also agree well with the ones presented in [41]. It indicates that the droplet behaves elastically.

\footnote{For interpretation of color in Fig. 1, the reader is referred to the web version of this article.}
4. Simulation of droplet formation in T-junction

A T-junction channel is considered in microscale having two inlets and one outlet as shown in Fig. 6. Two lengths of \( L_1 \) and \( L_2 \) are chosen to consider the computational efficiency as well as the droplet generation effect. The oil phase as the continuous phase is injected through the main channel, while the water phase as the dispersed phase is injected through the lateral channel. In the simulations, a constant velocity boundary scheme proposed by Zou and He [42] is imposed on the two inlets, and the open boundary condition [43] is adopted on the outlet. At the position where the fluids meet the solid walls, the half-way bounce-back boundary condition scheme is employed to achieve the non-slip boundary condition at the solid walls.

4.1. Effect of flow rate ratio

We study the effect of the flow rate ratio for two phase fluids. The physical value of the dispersed phase viscosity is fixed at \( \eta_d = 1 \times 10^{-3} \) Pa s. The physical value of density is \( \rho_d = \rho_c = 1000 \) kg/m\(^3\). Two different viscosity ratios \( \eta_d/\eta_c = 1/2 \) and \( 1/4 \) are used in the simulations, and the contact angle between the water droplet and channel walls is 180°. Garstecki et al. [19] pointed out that at low value of the capillary number, usually Ca < 10\(^{-2}\), the shear stress exerted on the interface of the emerging droplet could be ignored, and the squeezing pressure plays a dominant role for droplet breakup. The droplet blocks almost the entire cross-section of the main channel, leading to an increasing pressure in the upstream of the emerging droplet. The neck of the droplet squeezes at a rate proportional to the rate of the continuous fluids, and this growth, in turn, proceeds the droplet at a rate proportional to \( Q_d \). The head of the dispersed phase is elongated into the main channel until the neck of the dispersed phase becomes thin enough and consequently breaks up into a droplet. A single equation to the droplet length obeys a scaling law [19]

\[
L_{Wc} = 1 + a \frac{Q_d}{Q_c} - 1 = 1 + \frac{u_d \times W_d}{u_c \times W_c},
\]

(26)

where \( L \) is the length of dispersed droplet, \( W_c \) is the width of the main channel, and \( a \) is a constant of order one, whose particular value depends on the geometry of the T-junction. Fig. 7 shows droplet formation under different flow rate ratios. We can see that the length of the droplet is increased with the increasing flow rate of the dispersed phase at a fixed velocity of the continuous phase. Fig. 8 shows the simulation results and the scaling formula for the final length of the droplet. It indicates that, at the condition of the small capillary number of \( Ca = 0.005 \), the length of the droplet is dependent on the flow rate ratio of two phase fluids. However, it is independent of the viscosity ratio of two phase fluids. The length of the droplet increases linearly with the increasing flow rate ratio \( Q_d/Q_c \) by the fitting factor \( a = 2.0 \).

4.2. Effect of capillary number

The capillary number of the continuous phase is an important parameter to classify two-phase flow patterns in T-junction microchannels [11,18,19]. Xu et al. [18] found three typical flow regimes for the dispersed phase: squeezing regime (\( L > 2W_c \)), transient regime (\( W_c < L < 2W_c \)), and dripping regime (\( L < W_c \)), where \( W_c \) is the width of the main channel, and \( L \) is the length of the droplet. When the two-phase flow is in the squeezing regime, the tip of the dispersed fluid blocks almost the entire

![Fig. 5. Droplet under shear flow at Ca = 1.0 and breakup into two droplets at strains (a) \( \gamma t = 0 \), (b) \( \gamma t = 4 \), (c) \( \gamma t = 8 \), (d) \( \gamma t = 12 \), (e) \( \gamma t = 16 \), and (f) \( \gamma t = 20 \).](image-url)
cross-section of the main duct, hindering the flow of the continuous phase, thus a “plug-like” droplet is formed in the main channel. When the two-phase flow is in the transient regime, the dynamics of breakup are dominated by both the pressure drop across the droplet and the shear stress on the droplet. When the two-phase flow is in the dripping regime, the continuous phase flows faster through the gap between the droplet and the channel walls, hindering the flow of the continuous phase, thus a “plug-like” droplet is formed in the main channel. Fig. 9 shows the effect of \( \text{Ca} \) on the droplet detachment point. For the low capillary number, say, \( \text{Ca} = 0.0015 \), see Fig. 9(a), the droplet is pinched off at the corner of the T-junction, and the shear stress on the droplet is sufficiently large to cause the dispersed phase to pinch off at the T-junction microchannel. Fig. 9 shows the effect of \( \text{Ca} \) on the droplet detachment point. For the low capillary number, say, \( \text{Ca} = 0.0015 \), see Fig. 9(a), the droplet is pinched off at the corner of the T-junction, and the shear stress on the droplet is sufficiently large to cause the dispersed phase to pinch off at the T-junction microchannel. However, with the increase of \( \text{Ca} \), see Fig. 9(c), the dispersed phase is pulled downstream to form a longer laminar segment before the droplet breaks up. This result is also observed in both experiment [13] and simulations [11,44].

4.3. Effect of geometry

The length of the droplet would be influenced by the width ratio of the main channel \( W_c \) to lateral channel \( W_d \). We study various width ratios of \( W_d/W_c \). The contact angle between the water droplet and channel walls is \( 180^\circ \), i.e. the walls are hydrophobic. The densities of both phases are assumed to be unity and the viscosity ratio is \( \eta_d/\eta_c = 1/2 \).

As shown in Fig. 10, at the conditions of a fixed capillary number \( \text{Ca} = 0.006 \) and various velocity ratios, the droplet formation process (from left to right in each row) under three regimes with a fixed viscosity ratio \( \eta_d/\eta_c = 0.5 \) and a fixed flow rate ratio \( Q_d/Q_c = 0.5 \). (a) \( \text{Ca} = 0.0015 \), (b) \( \text{Ca} = 0.015 \), (c) \( \text{Ca} = 0.079 \).

4.4. Effect of wetting property

The contact angle \( \theta \) of the droplet in contact with the wall surface plays a significant role on the final length of the droplet at low capillary number. The most likely reason is that the size of the droplet is very large like a plug with a low capillary number, consequently, a large area of the droplet adheres to the channel walls, and the droplet generated in the hydrophobic walls is longer than in the less hydrophobic channel (compare Fig. 12(a) with (b)). However, this effect would diminish gradually with the increasing of the capillary number. When the two phase flow is in the dripping regime, the size of the droplet is small and only partially contacted with the channel wall, thus the hydrophilic walls are likely to obtain more water phase than the hydrophobic walls. For this reason, in an appropriate range of the contact angle, the length of the droplet generated in the less hydrophobic wetting conditions could be slightly larger than the droplet which is generated in the hydrophobic wetting conditions (see Fig. 12(c) and (d)). Meanwhile, an interesting phenomenon appears in the main channel that the advancing and receding contact angles of the droplet become different, and the shape of droplet gradually transforms from nearly spherical to pear-shaped (see Fig. 12(c)). However, in order to obtain approximate spherical droplets, the contact angle between the droplet and the channel walls should avoid setting too small. When the contact angle between the droplet and channel wall reaches \( 60^\circ \), a proximate semi-ellipse attaching to the upper wall of the channel is observed (see Fig. 12(e)) and when the contact angle between the droplet and the channel wall reaches \( 90^\circ \), a proximate rectangular droplet is generated in the microchannel (see Fig. 12(f)). In addition, when the capillary number reaches 0.1, droplets could not be generated in the both microchannels with \( 60^\circ \) and \( 90^\circ \) contact angles (see Fig. 12(g)).
and (h)). Fig. 13 shows the influence of the wetting properties of the channel walls on the droplet size as a function of the capillary number at a fixed viscosity ratio \( \frac{\nu_d}{\nu_c} = 1/2 \). It is remarkable that at low capillary numbers, smaller droplets are produced at the less hydrophobic wetting conditions while at high capillary numbers, slightly larger droplets are produced at the less hydrophobic wetting conditions. This result was also observed in numerical simulation by van der Graaf et al. [14].

5. Simulation of droplet formation in flow focusing structure

As we can see, due to dispersed phase squeezed into the confinement of the main channel, and the asymmetric geometry of the T-junction, the droplet generated by the T-junction channel is usually like a plug. Sometimes, we want to obtain a spherical droplet. A usually used axisymmetric device is the flow focusing, which has been widely used for generating highly spherical droplet [3,45–47]. Fig. 14 shows the flow focusing geometry implemented into a microfluidic device. In this structure, the dispersed phase flows in the middle of the channel, while the continuous phase flows through upper and lower channels. The continuous phase and dispersed phase penetrate into the downstream channel, and the continuous phase exerts pressure and stress which force the dispersed phase into a narrow thread. The dispersed phase breaks inside or downstream of the orifice, and then a spherical droplet is generated at the end of the flow stream where the neck forms.
The studied flow focusing structure is confined in a lattice system of $340 \times 80$ (see Fig. 14). In the simulations, a constant velocity boundary scheme proposed by Zou and He [42] is imposed on the left side. Open boundary conditions [43] are employed on the right side. At the position where the fluid meets the solid walls, half-way bounce-back boundary scheme is applied to achieve the non-slip velocity condition at the solid walls.

5.1. Effect of flow rate ratio

In this subsection, we use water as the dispersed phase and oil as the continuous phase, and observe a wide range of droplet size, which depends on the flow rate ratio of dispersed phase to continuous phase. The densities of the continuous and dispersed phase are assumed to be unity with $\eta_d/\eta_c = 1/2$ and $Ca = 0.036$. The channel surface is hydrophobic, i.e., the contact angle between dispersed phase and the channel surface is $180^\circ$. It is shown in Fig. 15 that the size of the droplet becomes large when the flow rate of the dispersed phase is growing with a fixed flow rate of the continuous phase. From Fig. 16, we find that the droplet diameter decreases as the viscosity ratio $\eta_d/\eta_c$ increases, which was also observed in the experiment [8]. Meanwhile, we observe that the generated droplets become highly monodisperse when the detachment point of the droplet in or close to the orifice. Emulsification occurred in this mode is called dripping mode, which is consistent with the observation in the experiment [9].

5.2. Effect of geometry

The geometry effect, i.e., the width of the orifice $D$ plays an important role in the final diameter of the droplets. From Fig. 17, we find that at the same conditions the wide orifice is likely to generate larger spherical droplet than the narrow orifice. When the flow rate ratio is large enough, here, equal to $2/3$, no droplet can be generated by the flow focusing configuration. Instead, a stable water jet appears in the centerline of the outlet channel. This flow pattern was also found by Anna et al. [3]. We compare the diameters of the droplets under the condition of three different flow rate ratios, see Fig. 18, and we find that three lines have the same linearity trend.

5.3. Effect of capillary number

The large capillary number will force the detachment point to move from the inside of the orifice to the downstream of the orifice, where it breaks into droplets, see Fig. 19(a–d). Emulsification occurred in this mode is called jetting mode, which produces a long jet that extends several times longer than the width of the orifice [9]. In some cases, the jetting type is unstable, resulting in polydisperse droplets when secondary or satellite droplets are accompanied with the main population of droplet. Hence, coalescence would occur downstream of the orifice when the secondary droplet...
catches up with the former one, see Fig. 20(a–d). The droplet coalescence can be reduced by using appropriate surfactant to stabilize the droplets. These observed results qualitatively agree with the experimental flow focusing studies [3,9,48].

6. Conclusions

We have simulated the droplets generation in two types of micro-devices, i.e., the T-junction microchannel and flow focusing configuration, based on the free energy model of the lattice Boltzmann method. Various parameters which affect the generation of the droplets, including the flow rate ratio, capillary number, geometry of configuration, and wetting properties of channel walls are systematically analyzed. It shows that the droplet size and shape depend on not only the fluid properties such as flow rate ratio, capillary number, but also the external flow conditions, i.e., geometry of configuration and wetting property of channel walls. The flow focusing configuration is likely to generate spherical droplet, while the T-junction is prone to generate elliptic droplet. High flow rate ratio lends to large diameter of droplet both in T-junction microchannel and flow focusing configuration. With the increasing of the capillary number, the detachment point of the droplet moves from the corner of T-junction or the orifice of flow focusing device to the downstream of the corner or the orifice, respectively. By considering the geometry of the T-junction microchannel and flow focusing configuration, we find that the T-junction microchannel with wide lateral channel generates droplet with large length and the flow focusing configuration with wide orifice is more likely to generate large diameter droplet. As for the wetting properties of the T-junction channel walls, the advancing and receding contact angles become different as the wetting property of the channel wall becomes more hydrophilic. In an appropriate range of the contact angle, it is observed that at low capillary number, smaller droplets are produced at the less hydrophobic wetting conditions, whereas at high capillary number, slightly larger droplets are produced at the less hydrophobic wetting conditions. The simulations are useful for understanding the droplet breakup in T-junction microchannel and flow focusing configuration. By adjusting the flow rate ratio, capillary number, geometry and wetting property of the device, we can easily obtain the favorite shape and size of the droplet. Furthermore, it is shown that the lattice Boltzmann method with free energy model is an effective way to simulate the generation of the droplets in T-junction microchannel as well as in flow focusing configuration.

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[13] Shen X, Zhang YH. Flow focusing configuration, and wetting properties of channel walls are systematically analyzed. It shows that the droplet size and shape depend on not only the fluid properties such as flow rate ratio, capillary number, but also the external flow conditions, i.e., geometry of configuration and wetting property of channel walls. The flow focusing configuration is likely to generate spherical droplet, while the T-junction is prone to generate elliptic droplet. High flow rate ratio lends to large diameter of droplet both in T-junction microchannel and flow focusing configuration. By adjusting the capillary number, the detachment point of the droplet moves from the corner of T-junction or the orifice of flow focusing device to the downstream of the corner or the orifice, respectively. By considering the geometry of the T-junction microchannel and flow focusing configuration, we find that the T-junction microchannel with wide lateral channel generates droplet with large length and the flow focusing configuration with wide orifice is more likely to generate large diameter droplet. As for the wetting properties of the T-junction channel walls, the advancing and receding contact angles become different as the wetting property of the channel wall becomes more hydrophilic. In an appropriate range of the contact angle, it is observed that at low capillary number, smaller droplets are produced at the less hydrophobic wetting conditions, whereas at high capillary number, slightly larger droplets are produced at the less hydrophobic wetting conditions. The simulations are useful for understanding the droplet breakup in T-junction microchannel and flow focusing configuration. By adjusting the flow rate ratio, capillary number, geometry and wetting property of the device, we can easily obtain the favorite shape and size of the droplet. Furthermore, it is shown that the lattice Boltzmann method with free energy model is an effective way to simulate the generation of the droplets in T-junction microchannel as well as in flow focusing configuration.


