Numerical simulation of droplet-based microfluidics

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Abstract: This paper discusses the features and applications of interface tracking techniques for modeling deroplet-based microfluidics. The paper reviews the state of the art of methods for tracking and capturing the interface. These methods are categorized as the implicit and the explicit methods. The implicit methods need to reconstruct the interface by reconnecting the markers on the interface. The implicit techniques implicitly describe the interface as a simple function. Thus, complicated topological changes of interface can be handled naturally and automatically. The implicit methods reviewed in this paper are the volume-of-fluid method, the phase-field method, the Lattice-Boltzmann method and the level-set method. The explicit methods mainly include the boundary-integral methods and the tracking methods.

Keywords: droplet-based microfluidics, boundary-integral method, tracking methods, volume-of-fluid method, level-set method

1. INTRODUCTION

Over the last few decades, modeling immiscible fluids such as oil and water has been a classical research topic. Droplet-based microfluidics presents a unique platform for mixing, reaction, separation, dispersion of drops and numerous other functions [1-4]. Droplet-based microfluidics is of great interest for biological research, chemical synthesis, drug delivery and medical diagnostics. Droplet-based microfluidics refers to devices and methods for controlling the fluid flows in length scales smaller than one millimeter. Monodisperse droplets in microfluidic devices have been generated using different microchannel configurations such as T-junction [5-6], flow focusing [7], or co-flowing [8]. The droplet size and the generation frequency can be accurately controlled by adjusting the flow rate ratio of the two phases, their viscosities and interfacial tension. In a microfluidics system, the effects of volume-based inertia and gravity do not play an important role as compared to the macroscale case. The surface-based interfacial tension and the viscosity dominate the behavior of multiphase flow in microscale. Numerical simulation is a powerful tool for understanding these complex multiphysics phenomena and the dynamics of a microfluidic system,

In general, the Navier-Stokes equations are solved numerically to obtain the velocity and pressure of fluid based on the established discretisation schemes such as the finite difference method (FDM), the finite volume method (FVM), or the finite element method (FEM). Recently, the Lattice Boltzmann method (LBM) is developed to solve the Navier-Stokes equations. However, the challenge in solving multiphase fluid flow problems is handling the interface separating the fluids involved and its evolution over time. The interface shape deforms continuously as two phases significantly affect each other as well as the boundary conditions on them. Nevertheless, special treatments need to deal with the property jump (or gradient) across the interface. A precise interface location needs to be determined.

Recently, different techniques were proposed for interface prediction. Traditionally, the interface that separates the two phases can be solved using volume-tracking method, front-tracking method, fractional volume of fluid (VOF), phase-field method, lattice Boltzmann method, the level-set method (LSM), and others. Slavov and Dimova categorized these methods into two types: explicit tracking methods and implicit tracking methods [9]. Explicit methods include boundary integral method, front tracking method and immersed interface method. Implicit ones include phase-field method and level-set method. The present review will be conducted to these categories. Cristini and Tan (2004) classified the methods into interface tracking methods and interface capturing methods based on whether the computational mesh or massless markers is attached on the interface [10]. The former includes boundary-integral methods, finite-element methods and immersed boundary methods. The latter includes lattice Boltzmann method, constrained-interpolation-profile, level-set, volume-of-fluid, coupled level-set, volume-of-fluid and partial-miscibility-model and phase-field methods. Garrioch and Baligo proposed to categorize these techniques as the moving font mesh to tack the interface and the fixed mesh to capture the interface location [11]. Each

categorization approach summarizes one of characters of the numerical methods of the interface prediction. For example, the level set method is an implicit, interface capturing and employing the fixed grid method.

2. PROBLEMS WITH MULTIPHASE SYSTEMS

Droplets Formation

Menech applied the phase-field method to model the breakup of a big droplet in a T-shaped junction [12]. The numerical results demonstrated that the droplet breakup region depends on the Capillary number (Ca), viscosity ratio ($\lambda = \mu_d / \mu_c$), and the initial drop dimension. Menech demonstrated that the numerical method can accurately describe the dynamics of a droplet. The same numerical method was used to investigate the different droplet formation regimes: squeezing, dripping and jetting. The regimes are distinguished by the capillary number Ca and the viscosity ratio λ. The results show that the droplet volume is strongly affected by the viscosity ratio. In a similar T-junction channel, lattice Boltzmann method was used to study the behavior of the droplet formation process [13-14]. Sang et al. (2009) employed the three-dimensional (3D) volume of fluid model (VOF) to study the impact of the viscosity of continuous phase on the droplet size and the frequency of the drop formation [15]. The numerical results agree well with the analytical results. The dynamics of droplet formation in the cross-junction configuration was numerically investigated by Wu et al. [16]using lattice Boltzmann method. The interfacial tension between two immiscible phases is calculated using the continuum surface force model (CSF). The simulation results of flow pattern, droplet size and velocity vectors agree well with the experimental results.

Droplets Behavior

The transport, merging, rupture, separating and colliding of droplets have also been modeled numerically [17-23]. Zheng and Zhang (2000) used level-set method to simulate the droplet spreading problems on the solid surface with solidification, which also involves a phase change process [24]. Recently, Takada et al. (2006) calculated the phenomenon of a droplet falling on the liquid film with the phase field method [25]. A ring-shaped vortex was captured during the droplet merging. Yap et al. employed the level set method to solve three coupling phases i.e. particle encapsulated droplets [26].

Actuated Droplets

The numerical methods also play an import role in the problems of droplet actuated by external forces. For example, the droplet can be controlled by a magnetic field or a temperature field described by the Maxwell equation or the energy equation, respectively. The droplet can also be squeezed or stretched by optical radiation pressure[46]. In the presence of a magnetic field, Korlie used a VOF model to simulate the bubbles rising in a ferrofluid and magnetic droplet falling down in a non-magnetic fluid [27]. Asimilar problems were solved by Ki et al. using level-set method[28]. Boundary element method and the finite element method were used to determine the equilibrium surface shapes of the ferrofluid drop[29]. Afkhami

et al. utilized the volume of fluid method to catch the shape of a droplet which was driven by an external permanent magnet in a cylindrical computational domain[30]. Among thermally mediated actuation problems, Tryggvason et al. considered the rising process of multiple bubbles in an initially quiescent fluid and under the influence of thermocapillary force [31]. Yap et al. solved the droplet breakup into two daughter droplets in the T-junction microchanel with the thermal mediated actuation [32].

Moving Contact Line Problems

The droplet evolution on a solid surface involving a triple phase line (gas, liquid and solid contact line) problems can also be solved numerically. Under a shear flow, Spelt numerically investigated a droplet rolling on a solid surface by adding the contact line velocity in the redistance function of level-set approach [33-34]. The level-set method coupled with the immersed interface method [35] or the volume-of-fluid method [36]can describe the motion of a sessile droplet on a planar surface. Ding and Spelt reported a good agreement between the level-set method and the diffuse interface method to solve the drop spreading problem [37].

3. EXPLICIT INTERFACE TRACKING METHOD

The interface is explicitly tracked either with a moving grid or massless markers seeded at the interface. Either a moving grid or a moving grid coupled the fixed grid is employed. Thus, the explicit method includes boundary integral method and front tracking method.

Boundary-Integral Method

In the boundary integral method, the evolution of a deformed droplet is calculated by time integrating the fluid velocity of a set of marker points on the interface [18]. The marker velocities are obtained by solving a boundary-integral equation instead of solving the velocity field. Thus, the interface is explicitly tracked. The flow solution is deduced from the information of the discrete points along the interface. The details of boundary integral method were reviewed by Pozrikidis [38]. The application and development of the method in multiphase fluid flow was reviewed by Hou et al. [39]. This review also discussed the numerical instability and the limited accuracy due to the involvement of the interfacial tension. However, the presented theory only based on a two-dimensional (2D) model. Actually, the previous 3D boundary integral method relying on fixed grid with uniform marker point density and cannot resolve the extreme changes of the interface during droplet breakup. To address this problem, an alternative method employing remeshing algorithms was proposed. These algorithms involve local mesh refinement and reconnection. Cristini et al. developed the adaptive dicretization algorithm to resolve the interface to fit the deformed drop shape [18]. The method was later refined by Cristini et al. based on the minimization of the mesh configurational

energy as the surface evolves[40]. The method was validated as accurate for test cases of drop breakup and coalescence. This work is followed by many papers with more 3D problems. The limit of numerical instability was overcome by the method proposed by Zinchenko et al. [41]. A special mesh stabilization method was utilized to solve the 3D extremely deformed interface. Further developments showed that this method is very successful in solving single droplet breakup [42], droplet squeezing among spheres [43], and optical stretching and squeezing of a sessile droplet [44].

Front Tracking Methods

The front tracking method was developed by Glimm's group and Tryggvason's group. Glimm presented a 3D front tracking algorithm to solve Rayleigh-Taylor instability problems [45]. Unverdi and Tryggvason investigated the rising of one and two bubbles[46]. This method needs connected markers to reconstruct the interface grid dynamically in the calculation process. The front grid moves through the fixed grid giving the precise location and the geometry of the interface. The interfacial tension is computed on the front and transfer to the fixed global grid. As discussed in [46], a separate unstructured triangular grid was introduced to mark the interface position while the computational domain is discretized by a regular fixed rectangular grid, Fig. (**1**). Naturally, the Navier-Stokes equations are solved on the fixed grid to control the motion of the multiphase system. It assumed that the fluid properties are constant in each phase. The interfacial jump condition is added to the momentum equations via a discrete delta function along the smooth interface. This multi-grid method shows that the front-tracking method is complex. Furthermore, this method can not solve thin film resulting from the droplet rupture. A topological change algorithm near the interface needs to be considered. Problems with topological changes involving breakup of drops and jet were investigated by Agresar et al. [47]. A pressure driven cell was modeled as a Newtonian micro droplet with constant surface tension. The topological change of the interface was added by Torres and Brackbill (2000) to solve the problem of coalescence of two spherical drops [22]. Esmaeeli and Tryggvason extended this approach to cases with phase change [48-49].

Recently, Mao showed with 2D conservative front-tracking method that the 2D discontinuity curves can be tracked in a 1D fashion [50]. Liu et al. presented a front tracking algorithm which can be applied uniformly to N dimensions [51]. Gois et al. proposed a new front-tracking method by advecting the unconnected points set [52]. The point set was used to mark the interface. The three-dimensional deformation of a spherical drop was modeled as the test case with topological changes. The improvement of the front tracking method was studied by Dijkhuizen et al. in the volume conservation and multiphase problems [53].

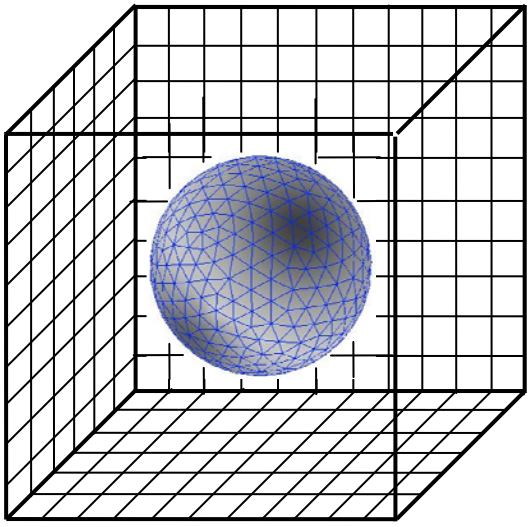

Fig. (1). The computational mesh. The 3D rectangular domain uses the uniform structure grid, and the interface uses a separate unstructured 2D grid.

4. IMPLICIT INTERFACE CAPTURING METHOD

The explicit method needs the stored points on the interface in order to reconstruct the interface. The interface resolution depends on the number of points. In the implicit method, a simple function is defined on a fixed grid to capture the interface. The interface location is approximated by the indicator function. Thus, both methods can not tell us where the exact interface location is. For *n*-dimensional problems, the explicit method use *n*-1 dimensional grid to reconstruct the interface, while the implicit method need resolve *n*-dimensional equation on the whole domain. The advantage of the implicit method is that it can solve more completed problems with topological changes. They include volume of fluid method, phase field method, lattice Boltzmann method, and level set method.

Volume of Fluid Method

A review of volume of fluid method (VOF) is given by Scardovelli and Zaleski [54]. Hirt and Nichols detailed the VOF techniques for interface capturing in non-uniform mesh [55]. In the VOF method, the volume fraction function is introduced and defined in a volume fraction field throughout the whole computational domain. The volume fraction function is $\frac{\partial \alpha}{\partial t} + \vec{u} \bullet \nabla \alpha = 0$ can be solved on a fixed-grid. Where α represents the volume fraction and has a value between 0 and 1. Figure (**2a**) shows a typical distribution of the volume fraction values. The values are reconstructed to find the interface location as shown in Fig. (**2b**). The interface lies within computational cell with a volume fraction function of $0< \alpha <1$, and the location of interface is 0.5. For a volume fraction function of unity, the computational cell is

completely filled with the primary phase. The computational cell is completely filled with the secondary phase in the case of volume fraction function of zero. To solve the function, the initial approximate interface position needs to be found. In addition, interface reconstruction should be carried out to determine the weighted density and viscosity for the computational cells and compute the volume flux for the convective terms in the governing equations. The crude reconstruction can generate a large error even with a simple velocity field such as translation or solid body rotation. The reconstruction methods include Simple Line Interface Construction (SLIC) reported by Noh and Woodward [56], Piecewise Linear Interface Construction (PLIC) with Lagrangian advection of the interface pieces by Gueyffier et al. [57], least-square fit with split Eulerian-Lagrangian advection by Scardovelli and Zaleski [58] and Parabolic Reconstruction of Surface Tension (PROST) employing piecewise parabolic curves by Renardy [59]. Rudman introduced flux-corrected transport (FCT) method for volume capturing and did not use interface reconstruction [60].

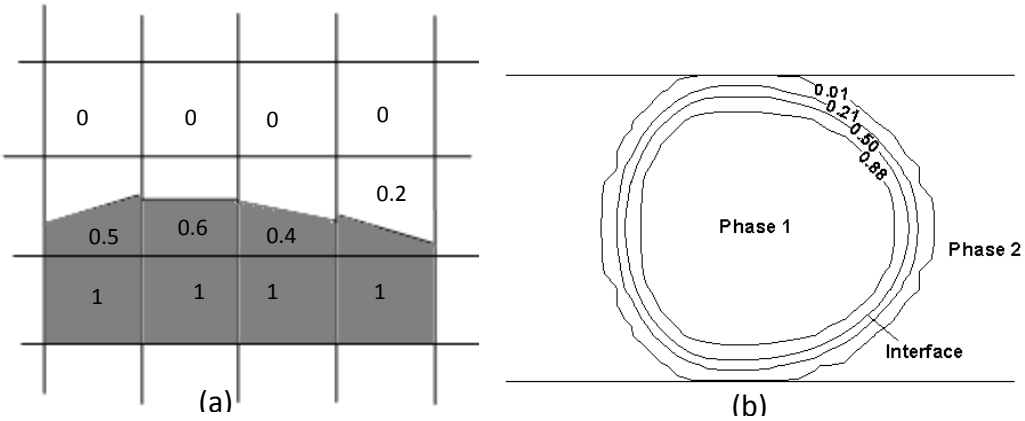

Fig. (2). (a) Volume fraction values; (b) Contour of volume fraction. α=0.01, α=0.21, α=0.5, and α=0.88.

After the interface reconstruction, the interface motion by the underlying flow field must be modeled by a suitable advection algorithm. The discretization of advection term is the main difficulty to guarantee the physical volume fraction distribution and the sharpness of the interface. The lower order scheme can smear the interface due to the numerical diffusion. A higher order scheme can result in numerical oscillations. Gopala et al. reviewed and discussed the advantages and limitations of several volume advection techniques [61] such as flux-corrected transport (FCT) algorithm [62], compressive interface capturing scheme (CICSAM)[63], gamma differencing scheme [64] and Lagrangian piecewise-linear interface reconstruction (L-PLIC) method [65]. The comparison was based on two practical test cases of sloshing of a liquid wave and the Rayleigh–Taylor instability problem. Recently, Park et al. employed a high resolution differencing schemes, Normalized Variable Diagram (NDV), to preserve the sharpness of interface and the boundedness of volume fraction [66].

The advantage of the VOF method is its superior volume or mass conservation of each fluid over other methods such as the level-set method. The interface could be captured implicitly, thus topological changes can be handled automatically. Problems with interfacial geometrical quantities such as the unit normal and the curvature can be encountered. These quantities are calculated from the volume fraction function which is nearly discontinuously distributed, and are important in the calculation of surface tension. It is not straight forward to calculate these quantities accurately. Fortunately, the level set method can fix this problem. As results, a number of researchers recently proposed a hybrid algorithm of coupling the level-set function with the VOF methods (CLSVOF) [67-69]. The VOF was used to reconstruct the interface, while the level-set function is used to calculate the interface and curvature. However, these methods are not easy to extend to three dimensions. Park et al. used NDV for the advection of the volume fraction function, and extended the CLSVOF method to multi-dimensional unstructured grid although the method is relatively complex [66]. The three-dimensional shape of a rising bubble in a liquid was tested.

The VOF method can exhibit the high accuracy in the calculation of three dimensional flows. Gueyffier et al. modeled a pinching pendant drop and found a good agreement with the experimental results [57]. Van der Pijl [70] and Sussman [69] calculated the problem of bubble rising in the liquid. Park et al. modeled droplets adhering to a vertical wall [66]. Wang et al.[71] modeled a water drop impact onto a deep water pool, wave breaking of a steep Stokes wave and plunging wave. The commercial software Fluent also employed VOF method to calculate multi-phase flow.

Phase-Field Method

One of the implicit methods for capturing the interface is phase-field method, which is also called the diffuse-interface method. In phase field method, a phase function $\phi(x,t)$ is introduced to represent the interface $\phi = 0$. Away from the interface, the function values of two phases are $\phi = +1$ and $\phi = -1$, respectively. The evolution of the phase-field function is governed by the Cahn-Hilliard equation [72], a fourth order nonlinear parabolic diffusion equation, it is $\phi_t + (\vec{u}\cdot)\phi = -\sigma\Delta[\Delta\phi - f(\phi)]$. The fnction $f(\phi)$ is a polynomial of ϕ [73]. Liu et al. used a Cahn-Hilliard equation to model coalescent of two bubbles [73]. Another alternative governing equation of the phase function is the Allen-Cahn type [74-75]. Because the phase-field method is a first order approximation to the sharp interface model, a fine grid is required around the interface.

The advantages and disadvantages of phase-field method are discussed by Slavov and Dimova [9]. This method can be easily extended to a three-dimensional problem, and has a straight-forward extension to arbitrary multi-phase systems [76]. Moreover, the method can handle the topological changes of the interface automatically. Adaptive moving mesh algorithm can be use to increase the efficiency and accuracy of the method [75]. This method requires an asymptotic analysis to be performed in order to obtain a mapping between the parameters of the phase field equations and the sharp interface equations. As

a result, the phase field model only reproduces the dynamics of the sharp interface equations with the limitation that the density difference is sufficiently small. Also a refined grid is needed to resolve the interface. In contrast, the level-set approach can be used to exactly locate the interface in a simple fashion. Recently, application of the method include multiple pinch-offs of a long cylindrical thread at small Reynolds number [77], droplet pinch-off in liquid/liquid jet configuration [78], and two drops coalescence evolving four phases [79].

Lattice Boltzmann Method

The lattice Boltzmann method (LBM) is a relatively new simulation technique. According to Takada et al. [25], the difference between phase field method and LBM only lies in the discretization to the Navier-Stokes equations. The method is successful in dealing with the interface tension and the complex boundaries with a large density ratio between the two phases. The lattice Boltzmann method constructs the kinetic equation of the discrete-velocity distribution function utilizing discrete lattice and discrete time. Thus, it is viewed as a special finite difference scheme for the kinetic equation. But LBM distinguishes itself from the conventional numerical schemes which are based on the discritization of the continuum equations. The LBM is a derivative of the lattice gas theory. A lattice gas theory consists of a regular lattice with particles residing on the nodes. As a result, the N-S equation can be derived from the lattice Boltzmann equation. The macroscopic dynamics of fluid is the behavior of the particles in the system.

An overview of the LBM was presented and discussed by Chen and Doolen [80]. This review discussed the different methods for modeling interfacial tension in a multiphase fluid flow: the free energy model and the interparticle interaction potential model. Lamura employed the first approach to simulate oil-water-surfactant mixtures [81]. The latter method was first proposed by Shan and Chen [82]. The third method, the He-Shan-Doolen method, was discussed by Nourgaliev et al. [83]. Nourgaliev et al also compared these three models, and their advantages and limitations. Sankaranarayanan et al. compared the simulation results of LBM and front tracking method based on the 2D bubble rising model [84]. The results showed that the BLM is not appropriate for low Mach number. Recently, LBM method becomes a popular modeling platform for droplet-based microfluidics. Van Der Graaf et al. (2006) [14] and Gupta and Kumar [13] used LBM to investigate the droplet formation process at a microfluidic T-junction. Wu et al. [16] used LBM to study the droplet formation process at the microfluidic cross-junction.

Level-Set Method

Osher and Sethian demonstrated a new algorithm of level set method to track the moving interface on the fixed-grid system [85]. The level set function $\phi(\vec{x},t)$ was introduced over the whole domain or near the interface and was defined as a signed shortest normal distance from the interface. The interface is implicitly represented by the zero level-set, $\phi(\vec{x},t)=0$. The values of $\phi(\vec{x},t)$ are positive inside the interface, and

negative outside the interface. The different signs distinguish the two different fluids. Figure (**3**) shows the typical contour of the level-set function. The values on the curves are the distance from the interface. By taking the time derivative of $\phi(\vec{x},t)=0$, the convection equation (level set equation) $\phi_t+\vec{u}\cdot\nabla\phi=0$ is used for calculating the motion of the interface. Fluid properties can be calculated from the level-set function through a smoothed Heaviside function.

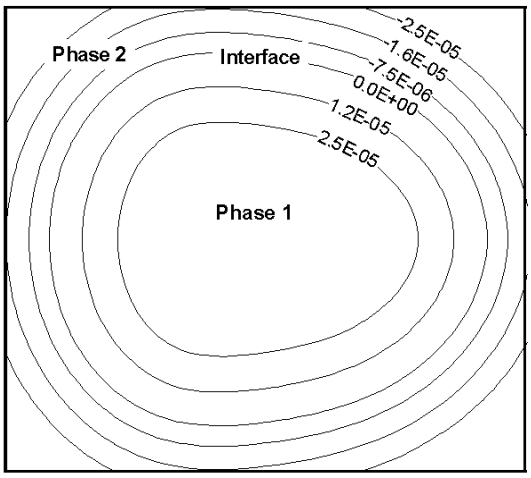

Fig. (3). The contour of level set function.

Currently, LSM has been used successfully for handling moving interface and free boundary problems in microfluidics [86]. Topological changes can be captured in a straightforward fashion, and thus the methods are readily implemented in both two and three spatial dimensions. We can conclude that LSM is a powerful tool to solve the complicated deformation and to construction of implicit surfaces on a fixed rectangular grid. The challenging problems such as coalescence/rupture of droplet and droplet falling down under difficult conditions can be simulated easily with the level set method.

Numerically, it is desirable to keep the level set function close to a signed distance function to the interface. However, the fact is the level set function will generally deviate from a signed distance function. Moreover, the discretization of the level set equation can cause numerical dissipation and inaccurate identification of interfaces. Flat or steep regions often occur near the interface. Generally, a reinitialization procedure is needed to reset the level set function to be a signed distance function to the interface with some degree of accuracy [20].

Normally, the level set and the reinitialization equations are evolved numerically by higher order advection schemes. They are two examples of a general Hamilton-Jacobi (HJ) equation $\phi_t+H(\nabla\phi)=0$. The detailed solution of this equation is well documented in the book by Osher and Fedkiw [87], which also include other higher order numerical discretiztion methods such as essentially non-oscillatory (ENO) and

weighted essentially nonoscillatory (WENO). The gain in accuracy of on the higher order schemes is compromised by the long time integration, which is not desirable. Therefore, new techniques need to be developed to reduce the computational time. Solving the level set function in the global domain wastes computing resources and times, because only the domain near the interface is of interest. Peng et al. introduced an approach that only solves the level-set function within a band $|\phi(\vec{x})| < \gamma$ near the interface, where γ is width of the interface [88]. This method does not compromise the accuracy since the level-set value is important only around the interface. Figure (**4**) shows the marked region of the interface, the computational domain of the level set function and the reinitialize function. This tremendous time saving can reduce one order of computational effort. Peng et al. successfully solved the problems of vortex sheet and bubble separation.

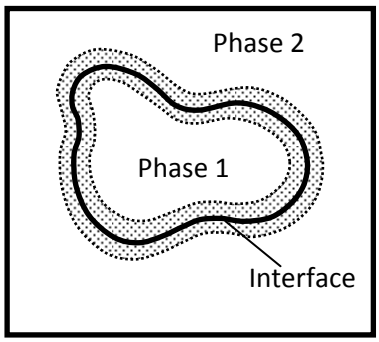

Fig. (4). The band of computational domain for level set equation and reinitialization equation.

Even using the higher-order advection schemes to evolve the level-set equation, the mass error still cannot be avoided. Figure (5) depicts the typical examples of mass error. The error is caused because the sharpness of the interface is destroyed by under-resolved regions during the discretisation process. This mass conservation problem can be solved by many methods. One method employs the re-initialization equation as mentioned above. The details of this method are discussed by Sussman et al. Another different reinitialization procedure was introduced by Chang et al. [89] who solved the equation $\phi_t + \Delta A\left(-P+\kappa\right)\left|\nabla\phi\right| = 0$ to the steady state, where ΔA is the difference of the mass between initial mass and the mass in the droplet deforming process. P is constant, and κ is curvature. Unfortunately, this improvement in the mass conservation cannot solve the mass imbalance problem of the level set method [89]. Therefore, a global mass correction technique is needed [26, 90]. A correction is added to the level-set equation in order to preserve the initial mass. Mass is conserved in a global sense. Actually, most researchers agree that employing the particle level-set method can improve mass conservation. A number of particles are seeded into the grid cell to track the characteristic information, and thus can accurately reconstruct the interface where the level set method failed to preserve mass. Traditionally, the particles are

placed throughout the fluid domain and move with the local velocity [91-92]. This method is successful in solving the free surface problems i.e. falling free surface, splashing of water, and water sloshing in a tank. Enright et al. proposed a new numerical method [93] that seeds Lagrangian marker particles within a narrow band around the interface. First, the initial particles seeded randomly into the cells. Then these particles are attracted to its corresponding region after a simple attraction procedure. While the negative particles are attracted to the $\phi < 0$ region, the positive particles are attracted to the $\phi > 0$ region as shown in the example of Fig. (6). Enright et al. (2002)[93], Wang et al. (2009) [94] and Tran et al. (2004) [95] proposed particle correction strategies to guarantee that the particles do not escape across the interface. The last procedure to be carried out is particle reseeding, when there are not enough particles in some region to resolve the interface well after few iterations [94]. Fig. (7) shows one case of the particle poor distribution around the interface. However, reseeding algorithm is not a perfect method to smooth the interface. It is necessary to randomly seed and attract the particles repeatedly when the reseeding algorithm failed to maintain the smoothness of the interface.

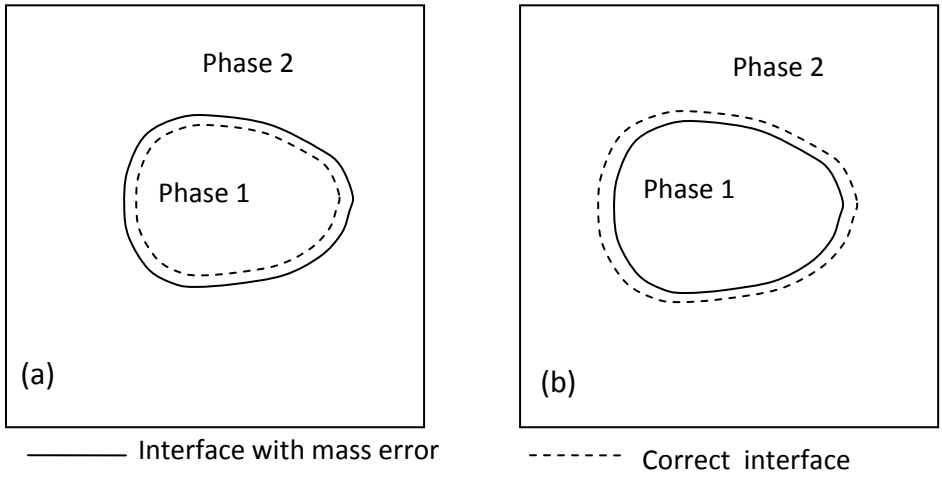

Fig. (5). Mass error in the level set method: (a) mass loss; (b) mass surplus.

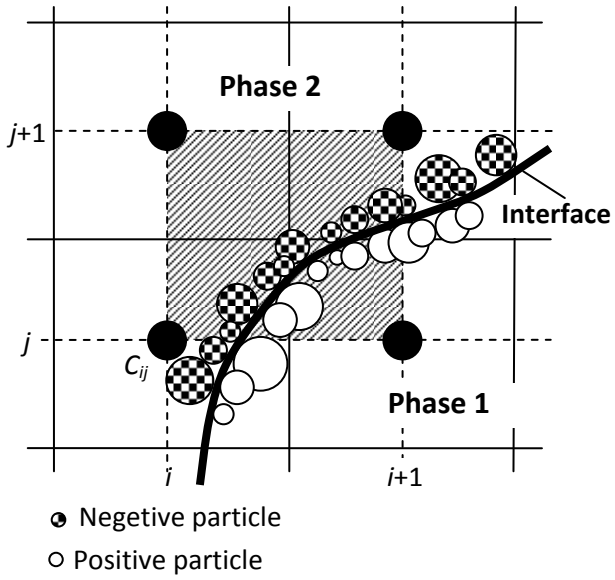

Fig. (6). Some of the particles with radius assigned after attraction procedure.

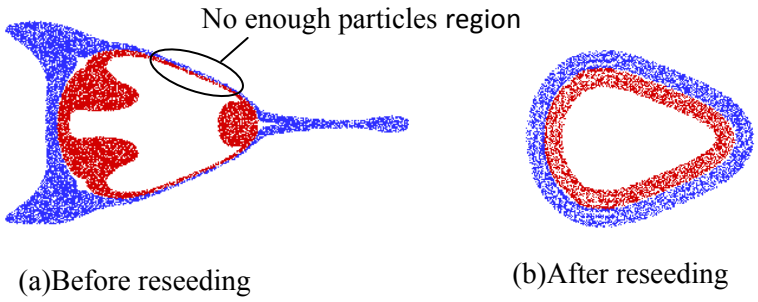

Fig. (7). Particle reseeding. Red ones are positive particles, and blue ones are negative particles.

Recently, level-set methods have been used quite successfully in moving interface as well as multiphase flow in two- or three-dimensional problems: particle-encapsulated droplet transporting in the fluid flow [86], droplet spreading and solidification [24], bubble rising and growth in a stationary fluid [96], droplet falling down[97], and bubble adhering to the solid surface in the fluid [98], topological changes of the interface such as droplet pinching and connection [99], droplet collision and membrane break [100], breakup into smaller droplets [101]. In the field of the droplet based microfluidics, numerical simulation with level-set method has the potential to play an important role.

5. CONCLUSION

This paper reviews the theory and applications of the different interface tracking and capturing methods for droplet-based microfluidics. In a multipase fluid flow, it is difficult to numerically simulate the interface

because of the jump of properties and the moving interface. Moreover, the capillary force, shear stress, interfacial tension, or other external forces are strongly coupled. Thus, the interface movement needs to be linked with the discretization of the velocity field and the properties of fluids to model challenging problems such as droplet breakup and coalescence. We reviewed here the successful methods in handling the complicated interface deformation. The review would help the readers to have an overview on the available techniques for modeling droplet-based microfluidics.

REFERENCES

[1] Burns, M.A.;Mastrangelo, C.H.;Sammarco, T.S.;Man, F.P.;Webster, J.R.;Johnson, B.N.;Foerster, B.;Jones, D.;Fields, Y.;Kaiser, A.R.;Burke, D.T. Microfabricated structures for integrated DNA analysis. *Proc. Nat. Acad. Sci. U.S.A.*, **1996**, 93(11), 5556-5561.

[2] Cho, S.K.;Moon, H.;Kim, C.J. Creating, transporting, cutting, and merging liquid droplets by electrowetting-based actuation for digital microfluidic circuits. *J. Microelectromech. Syst.*, **2003**, 12(1), 70-80.

[3] Fidalgo, L.M.;Abell, C.;Huck, W.T.S. Surface-induced droplet fusion in microfluidic devices. *Lab Chip*, **2007**, 7(8), 984-986.

[4] Lehmann, U.;Hadjidj, S.;Parashar, V.K.;Vandevyver, C.;Rida, A.;Gijs, M.A.M. Two-dimensional magnetic manipulation of microdroplets on a chip as a platform for bioanalytical applications. *Sens. Actuators, B*, **2006**, 117(2), 457-463.

[5] Garstecki, P.;Fuerstman, M.J.;Stone, H.A.;Whitesides, G.M. Formation of droplets and bubbles in a microfluidic T-junction - Scaling and mechanism of break-up. *Lab Chip*, **2006**, 6(3), 437-446.

[6] Xu, J.H.;Li, S.W.;Tán, J.;Wang, Y.J.;Luo, G.S. Preparation of highly monodisperse droplet in a T-junction microfluidic device. *AIChE J.*, **2006**, 52(9), 3005-3010.

[7] Nguyen, N.T.;Ting, T.H.;Yap, Y.F.;Wong, T.N.;Chai, J.C.K.;Ong, W.L.;Zhou, J.;Tan, S.H.;Yobas, L. Thermally mediated droplet formation in microchannels. *Appl. Phys. Lett.*, **2007**, 91(8).

[8] Xu, J.H.;Li, S.W.;Lan, W.J.;Luo, G.S. Microfluidic approach for rapid interfacial tension measurement. *Langmuir*, **2008**, 24(19), 11287-11292.

[9] Slavov, V.;Dimova, S. *Phase-field versus level set method for 2D dendritic growth*. 2007.

[10] Cristini, V.;Tan, Y.C. Theory and numerical simulation of droplet dynamics in complex flows - A review. *Lab Chip*, **2004**, 4(4), 257-264.

[11] Garrioch, S.H.;Baliga, B.R. A PLIC volume tracking method for the simulation of two-fluid flows. *Int. J. Numer. Methods Fluids*, **2006**, 52(10), 1093-1134.

[12] De Menech, M. Modeling of droplet breakup in a microfluidic T-shaped junction with a phase-field model. *Physical Review E - Statistical, Nonlinear, and Soft Matter Physics*, **2006**, 73(3), 1-9.

[13] Gupta, A.;Kumar, R. Effect of geometry on droplet formation in the squeezing regime in a microfluidic T-junction. *Microfluid. Nanofluid.*, **2010**, 8(6), 799-812.

[14] Van Der Graaf, S.;Nisisako, T.;Schroën, C.G.P.H.;Van Der Sman, R.G.M.;Boom, R.M. Lattice Boltzmann simulations of droplet formation in a T-shaped microchannel. *Langmuir*, **2006**, 22(9), 4144-4152.

[15] Sang, L.;Hong, Y.;Wang, F. Investigation of viscosity effect on droplet formation in T-shaped microchannels by numerical and analytical methods. *Microfluid. Nanofluid.*, **2009**, 6(5), 621-635.

[16] Wu, L.;Tsutahara, M.;Kim, L.S.;Ha, M. Three-dimensional lattice Boltzmann simulations of droplet formation in a cross-junction microchannel. *Int. J. Multiphase Flow*, **2008**, 34(9), 852-864.

[17] Coulliette, C.;Pozrikidis, C. Motion of an array of drops through a cylindrical tube. *J. Fluid Mech.*, **1998**, 358, 1-28.

[18] Cristini, V.;Bławzdziewicz, J.;Loewenberg, M. Drop breakup in three-dimensional viscous flows. *Phys. Fluids*, **1998**, 10(8), 1781-1783.

[19] Quan, S.;Lou, J.;Schmidt, D.P. Modeling merging and breakup in the moving mesh interface tracking method for multiphase flow simulations. *J. Comput. Phys.*, **2009**, 228(7), 2660-2675.

[20] Sussman, M. A level set approach for computing solutions to incompressible two-phase flow. *J. Comput. Phys.*, **1994**, 114(1), 146-159.

[21] Sussman, M.;Fatemi, E. Efficient, interface-preserving level set redistancing algorithm and its application to interfacial incompressible fluid flow. *SIAM J. Sci. Comput.*, **1999**, 20(4), 1165-1191.
[22] Torres, D.J.;Brackbill, J.U. The Point-Set Method: Front-Tracking without Connectivity. *J. Comput. Phys.*, **2000**, 165(2), 620-644.
[23] Zhang, H.;Zheng, L.L.;Prasad, V.;Hou, T.Y. A curvilinear level set formulation for highly deformable free surface problems with application to solidification. *Numer. Heat Transfer, Part B*, **1998**, 34(1), 1-20.
[24] Zheng, L.L.;Zhang, H. An adaptive level set method for moving-boundary problems: Application to droplet spreading and solidification. *Numer. Heat Transfer, Part B*, **2000**, 37(1-4), 437-454.
[25] Takada, N.;Misawa, M.;Tomiyama, A. A phase-field method for interface-tracking simulation of two-phase flows. *Math. Comput. Simul*, **2006**, 72(2-6), 220-226.
[26] Yap, Y.F.;Chai, J.C.;Wong, T.N.;Toh, K.C.;Zhang, H.Y. A global mass correction scheme for the level-set method. *Numer. Heat Transfer, Part B*, **2006**, 50(5), 455-472.
[27] Korlie, M.S.;Mukherjee, A.;Nita, B.G.;Stevens, J.G.;Trubatch, A.D.;Yecko, P. Modeling bubbles and droplets in magnetic fluids. *J. Phys. Condens. Matter*, **2008**, 20(20).
[28] Ki, H. Level set method for two-phase incompressible flows under magnetic fields. *Comput. Phys. Commun.*, **2010**, 181(6), 999-1007.
[29] Lavrova, O.;Matthies, G.;Mitkova, T.;Polevikov, V.;Tobiska, L. Numerical treatment of free surface problems in ferrohydrodynamics. *J. Phys. Condens. Matter*, **2006**, 18(38), S2657-S2669.
[30] Afkhami, S.;Renardy, Y.;Renardy, M.;Riffle, J.S.;St Perre, T. Field-induced motion of ferrofluid droplets through immiscible viscous media. *J. Fluid Mech.*, **2008**, 610, 363-380.
[31] Tryggvason, G.;Bunner, B.;Esmaeeli, A.;Juric, D.;Al-Rawahi, N.;Tauber, W.;Han, J.;Nas, S.;Jan, Y.J. A Front-Tracking Method for the Computations of Multiphase Flow. *J. Comput. Phys.*, **2001**, 169(2), 708-759.
[32] Yap, Y.F.;Tan, S.H.;Nguyen, N.T.;Murshed, S.M.S.;Wong, T.N.;Yobas, L. Thermally mediated control of liquid microdroplets at a bifurcation. *J. Phys. D: Appl. Phys.*, **2009**, 42(6).
[33] Spelt, P.D.M. A level-set approach for simulations of flows with multiple moving contact lines with hysteresis. *J. Comput. Phys.*, **2005**, 207(2), 389-404.
[34] Spelt, P.D.M. Shear flow past two-dimensional droplets pinned or moving on an adhering channel wall at moderate Reynolds numbers: A numerical study. *J. Fluid Mech.*, **2006**, 561, 439-463.
[35] Hunter, J.K.;Li, Z.;Zhao, H. Reactive autophobic spreading of drops. *J. Comput. Phys.*, **2002**, 183(2), 335-366.
[36] Yokoi, K.;Vadillo, D.;Hinch, J.;Hutchings, I. Numerical studies of the influence of the dynamic contact angle on a droplet impacting on a dry surface. *Phys. Fluids*, **2009**, 21(7).
[37] Ding, H.;Spelt, P.D.M. Inertial effects in droplet spreading: A comparison between diffuse-interface and level-set simulations. *J. Fluid Mech.*, **2007**, 576, 287-296.
[38] Pozrikidis, C. Interfacial dynamics for Stokes flow. *J. Comput. Phys.*, **2001**, 169(2), 250-301.
[39] Hou, T.Y.;Lowengrub, J.S.;Shelley, M.J. Boundary Integral Methods for Multicomponent Fluids and Multiphase Materials. *J. Comput. Phys.*, **2001**, 169(2), 302-362.
[40] Cristini, V.;Blawzdziewicz, J.;Loewenberg, M. An Adaptive Mesh Algorithm for Evolving Surfaces: Simulations of Drop Breakup and Coalescence. *J. Comput. Phys.*, **2001**, 168(2), 445-463.
[41] Zinchenko, A.Z.;Rother, M.A.;Davis, R.H. Cusping, capture, and breakup of interacting drops by a curvatureless boundary-integral algorithm. *J. Fluid Mech.*, **1999**, 391, 249-292.
[42] Janssen, P.A.;Anderson, P.D. Boundary-integral method for drop deformation between parallel plates. *Phys. Fluids*, **2007**, 19(4).
[43] Zinchenko, A.Z.;Davis, R.H. Boundary-integral algorithm for drop squeezing through a granular material. *AIP Conference Proceedings*, **2008**, 973, 652-657.
[44] Chraïbi, H.;Lasseux, D.;Arquis, E.;Wunenburger, R.;Delville, J.P. Stretching and squeezing of sessile dielectric drops by the optical radiation pressure. *Physical Review E - Statistical, Nonlinear, and Soft Matter Physics*, **2008**, 77(6).
[45] Glimm, J.;Grove, J.W.;Li, X.L.;Shyue, K.M.;Zeng, Y.;Zhang, Q. Three-dimensional front tracking. *SIAM J. Sci. Comput.*, **1998**, 19(3), 703-727.
[46] Unverdi, S.O. A front-tracking method for viscous, incompressible, multifluid flows. *J. Comput. Phys.*, **1992**, 100(1), 25-37.

[47] Agresar, G.;Linderman, J.J.;Tryggvason, G.;Powell, K.G. An Adaptive, Cartesian, Front-Tracking Method for the Motion, Deformation and Adhesion of Circulating Cells. *J. Comput. Phys.*, **1998**, 143(2), 346-380.
[48] Esmaeeli, A.;Tryggvason, G. Computations of Explosive Boiling in Microgravity. *J. Sci. Comput.*, **2003**, 19(1-3), 163-182.
[49] Esmaeeli, A.;Tryggvason, G. Computations of film boiling. Part I: Numerical method. *Int. J. Heat Mass Transfer*, **2004**, 47(25), 5451-5461.
[50] Mao, D.k. Towards front-tracking based on conservation in two space dimensions II, tracking discontinuities in capturing fashion. *J. Comput. Phys.*, **2007**, 226(2), 1550-1588.
[51] Liu, J.;Lim, H.K.;Glimm, J.;Li, X. A conservative front tracking method in N-dimensions. *J. Sci. Comput.*, **2007**, 31(1-2), 213-236.
[52] Gois, J.P.;Nakano, A.;Nonato, L.G.;Buscaglia, G.C. Front tracking with moving-least-squares surfaces. *J. Comput. Phys.*, **2008**, 227(22), 9643-9669.
[53] Dijkhuizen, W.;Roghair, I.;Annaland, M.V.S.;Kuipers, J.A.M. DNS of gas bubbles behaviour using an improved 3D front tracking model-Model development. *Chem. Eng. Sci.*, **2010**, 65(4), 1427-1437.
[54] Scardovelli, R.;Zaleski, S. Direct numerical simulation of free-surface and interfacial flow. *Annu. Rev. Fluid Mech.*, **1999**, 31, 567-603.
[55] Hirt, C.W.;Nichols, B.D. Volume of fluid (VOF) method for the dynamics of free boundaries. *J. Comput. Phys.*, **1981**, 39(1), 201-225.
[56] Noh, W.;Woodward, P. SLIC-simple line interface calculation *International Conference on Fluid Dynamics*, **1976**, 59, 330-340.
[57] Gueyffier, D.;Li, J.;Nadim, A.;Scardovelli, R.;Zaleski, S. Volume-of-Fluid Interface Tracking with Smoothed Surface Stress Methods for Three-Dimensional Flows. *J. Comput. Phys.*, **1999**, 152(2), 423-456.
[58] Scardovelli, R.;Zaleski, S. Interface reconstruction with least-square fit and split Eulerian-Lagrangian advection. *Int. J. Numer. Methods Fluids*, **2003**, 41(3), 251-274.
[59] Renardy, Y.;Renardy, M. PROST: A parabolic reconstruction of surface tension for the volume-of-fluid method. *J. Comput. Phys.*, **2002**, 183(2), 400-421.
[60] Rudman, M. Volume-tracking methods for interfacial flow calculations. *Int. J. Numer. Methods Fluids*, **1997**, 24(7), 671-691.
[61] Gopala, V.R.;van Wachem, B.G.M. Volume of fluid methods for immiscible-fluid and free-surface flows. *Chem. Eng. J.*, **2008**, 141(1-3), 204-221.
[62] Boris, J.P.;Book, D.L. Flux-corrected transport. I. SHASTA, a fluid transport algorithm that works. *J. Comput. Phys.*, **1973**, 11(1), 38-69.
[63] Ubbink, O.;Issa, R.I. A Method for Capturing Sharp Fluid Interfaces on Arbitrary Meshes. *J. Comput. Phys.*, **1999**, 153(1), 26-50.
[64] Jasak, H.;Weller, H.G.;Gosman, A.D. High resolution NVD differencing scheme for arbitrarily unstructured meshes. *Int. J. Numer. Methods Fluids*, **1999**, 31(2), 431-449.
[65] Van Wachem, B.G.M.;Schouten, J.C. Experimental validation of 3-D Lagrangian VOF model: Bubble shape and rise velocity. *AIChE J.*, **2002**, 48(12), 2744-2753.
[66] Park, I.R.;Kim, K.S.;Kim, J.;Van, S.H. A volume-of-fluid method for incompressible free surface flows. *Int. J. Numer. Methods Fluids*, **2009**, 61(12), 1331-1362.
[67] Son, G. Efficient implementation of a coupled level-set and volume-of-fluid method for three-dimensional incompressible two-phase flows. *Numer. Heat Transfer, Part B*, **2003**, 43(6), 549-565.
[68] Sussman, M.;Puckett, E.G. A Coupled Level Set and Volume-of-Fluid Method for Computing 3D and Axisymmetric Incompressible Two-Phase Flows. *J. Comput. Phys.*, **2000**, 162(2), 301-337.
[69] Sussman, M.;Smith, K.M.;Hussaini, M.Y.;Ohta, M.;Zhi-Wei, R. A sharp interface method for incompressible two-phase flows. *J. Comput. Phys.*, **2007**, 221(2), 469-505.
[70] van der Pijl, S.P.;Segal, A.;Vuik, C.;Wesseling, P. A mass-conserving Level-Set method for modelling of multi-phase flows. *Int. J. Numer. Methods Fluids*, **2005**, 47(4), 339-361.
[71] Wang, Z.;Yang, J.;Koo, B.;Stern, F. A coupled level set and volume-of-fluid method for sharp interface simulation of plunging breaking waves. *Int. J. Multiphase Flow*, **2009**, 35(3), 227-246.
[72] Cahn, J.W.;Hilliard, J.E. Free energy of a nonuniform system. III. Nucleation in a two-component incompressible fluid. *J. Chem. Phys.*, **1959**, 31(3), 688-699.

[73] Liu, C.;Shen, J. A phase field model for the mixture of two incompressible fluids and its approximation by a Fourier-spectral method. *Physica D*, **2003**, 179(3-4), 211-228.
[74] Liu, C.;Walkington, N.J. An Eulerian description of fluids containing visco-elastic particles. *Arch. Ration. Mech. Anal.*, **2001**, 159(3), 229-252.
[75] Zhang, Z.;Tang, H. An adaptive phase field method for the mixture of two incompressible fluids. *Comput. Fluids*, **2007**, 36(8), 1307-1318.
[76] Kim, J.;Kang, K.;Lowengrub, J. Conservative multigrid methods for Cahn-Hilliard fluids. *J. Comput. Phys.*, **2004**, 193(2), 511-543.
[77] Kim, J. A diffuse-interface model for axisymmetric immiscible two-phase flow. *Appl. Math. Comput.*, **2005**, 160(2), 589-606.
[78] Kim, C.H.;Shin, S.H.;Lee, H.G.;Kim, J. Phase-field model for the pinchoff of liquid-liquid jets. *J. Korean Phys. Soc.*, **2009**, 55(4), 1451-1460.
[79] Kim, J. A generalized continuous surface tension force formulation for phase-field models for multi-component immiscible fluid flows. *Comput. Meth. Appl. Mech. Eng.*, **2009**, 198(37-40), 3105-3112.
[80] Chen, S.;Doolen, G.D. Lattice Boltzmann model for fluid flows. *Annu. Rev. Fluid. Mech.* , **1998**, 30, 329-364.
[81] Lamura, A.;Gonnella, G.;Yeomans, J.M. A lattice Boltzmann model of ternary fluid mixtures. *Europhys. Lett.*, **1999**, 45(3), 314-320.
[82] Shan, X.;Chen, H. Lattice Boltzmann model for simulating flows with multiple phases and components. *Phys. Rev. E*, **1993**, 47(3), 1815-1819.
[83] Nourgaliev, R.R.;Dinh, T.N.;Theofanous, T.G.;Joseph, D. The lattice Boltzmann equation method: Theoretical interpretation, numerics and implications. *Int. J. Multiphase Flow*, **2003**, 29(1), 117-169.
[84] Sankaranarayanan, K.;Kevrekidis, I.G.;Sundaresan, S.;Lu, J.;Tryggvason, G. A comparative study of lattice Boltzman and front-trancking finite-difference methods for bubble simulations. *Int. J. Multiphase Flow*, **2003**, 29(1), 109-116.
[85] Osher, S.;Sethian, J.A. Fronts propagating with curvature-dependent speed: Algorithms based on Hamilton-Jacobi formulations. *J. Comput. Phys.*, **1988**, 79(1), 12-49.
[86] Yap, Y.F.;Chai, J.C.;Wong, T.N.;Nguyen, N.T.;Toh, K.C.;Zhang, H.Y.;Yobas, L. A procedure for the motion of particle-encapsulated droplets in microchannels. *Numer. Heat Transfer, Part B*, **2008**, 53(1), 59-74.
[87] Osher, S.;Fedkiw, R.P. Level set methods and dynamic implicit surfaces *Spring*, New York, 2003.
[88] Peng, D.;Merriman, B.;Osher, S.;Zhao, H.;Kang, M. A PDE-Based Fast Local Level Set Method. *J. Comput. Phys.*, **1999**, 155(2), 410-438.
[89] Chang, Y.C.;Hou, T.Y.;Merriman, B.;Osher, S. A level set formulation of Eulerian interface capturing methods for incompressible fluid flows. *J. Comput. Phys.*, **1996**, 124(2), 449-464.
[90] Lakehal, D.;Meier, M.;Fulgosi, M. Interface tracking towards the direct simulation of heat and mass transfer in multiphase flows. *Int. J. Heat Fluid Flow*, **2002**, 23(3), 242-257.
[91] Harlow, F.H.;Welch, J.E. Numerical calculation of time-dependent viscous incompressible flow of fluid with free surface. *Phys. Fluids*, **1965**, 8(12), 2182-2189.
[92] Chen, S.;Johnson, D.B.;Raad, P.E.;Fadda, D. The surface marker and micro cell method. *Int. J. Numer. Methods Fluids*, **1997**, 25(7), 749-778.
[93] Enright, D.;Fedkiw, R.;Ferziger, J.;Mitchell, I. A hybrid particle level set method for improved interface capturing. *J. Comput. Phys.*, **2002**, 183(1), 83-116.
[94] Wang, Z.;Yang, J.;Stern, F. An improved particle correction procedure for the particle level set method. *J. Comput. Phys.*, **2009**, 228(16), 5819-5837.
[95] Tran, L.B.;Udaykumar, H.S. A particle-level set-based sharp interface cartesian grid method for impact, penetration, and void collapse. *J. Comput. Phys.*, **2004**, 193(2), 469-510.
[96] Son, G. A numerical method for incompressible two-phase flows with open or periodic boundaries. *Numer. Heat Transfer, Part B*, **2001**, 39(1), 45-60.
[97] Ni, M.J.;Abdou, M.;Komori, S. A variable-density projection method for interfacial flows. *Numer. Heat Transfer, Part B*, **2003**, 44(6), 553-574.
[98] Son, G. A level set method for incompressible two-fluid flows with immersed solid boundaries. *Numer. Heat Transfer, Part B*, **2005**, 47(5), 473-489.

[99] Nochetto, R.H.;Walker, S.W. A hybrid variational front tracking-level set mesh generator for problems exhibiting large deformations and topological changes. *J. Comput. Phys.*, **2010**, 229(18), 6243-6269.
[100] Tanguy, S.;Berlemont, A. Application of a level set method for simulation of droplet collisions. *Int. J. Multiphase Flow*, **2005**, 31(9), 1015-1035.
[101] Croce, R.;Griebel, M.;Schweitzer, M.A. Numerical simulation of bubble and droplet deformation by a level set approach with surface tension in three dimensions. *Int. J. Numer. Methods Fluids*, **2010**, 62(9), 963-993.