SIMULATION OF THE COALESCENCE OF DROPLETS EMPLOYING LATTICE BOLTZMANN AND LEVEL SET METHODS

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Abstract

A hybrid lattice Boltzmann and level set method (LBLSM) for two-phase immiscible fluids with large density differences is proposed, where the two fluids are assumed incompressible. The common Navier-Stokes incompressible equations are replaced by lattice Boltzmann method for calculating the velocities of the domain. The interface of the two fluids is captured by the level set function that is a robust technique for capturing sophisticated changes in geometry and topology. The surface tension force is replaced by an equivalent force field which is proportional to the curvature of the interface and the experimental coefficient of surface tension. The method can be applied to simulate two-phase fluid flows with density ratio up to 1000 and viscosity ratio up to 100. In case of zero or known pressure gradient the method is completely explicit. Assuming zero pressure gradient, the coalescence of two droplets is simulated. Besides, the entrapment of a small bubble between the interfaces of the two droplets was also captured in the simulation. The results are in agreement with experimental results, so the new method (LBLSM) is valid for simulation of droplet phenomena. Afterwards the coalescence of three droplets is simulated and the evolution of the droplets in a proposed time scale is investigated.

Keywords: Lattice Boltzmann method; Level set method; droplet coalescence.

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1 Introduction

Multiphase flows are widely used in many fields such as petroleum engineering, nuclear engineering, sprays, wave mechanics, bubble dynamics, bio engineering and combustion. Developing a method for simulation of various types of multiphase flows is one of the most important engineering challenges. In case of large density differences across the interface, due to the significant role of the forces between the components, the complexity of the simulation doubles.

Collision dynamics of two droplets is one of the most fascinating and also sophisticated problems in computational fluid mechanics. The phenomenon of binary coalescence, in which two droplets merge and form a single droplet, is an essential feature in many natural and industrial processes and therefore its simulation may be extensively used in various phenomena such as spray coating, hydrocarbon fermentation and waste treatment [1-2].

Several methods have been used for modeling of multiphase flows. They are divided into "front/interface tracking" and "front/interface capturing" methods. In front tracking the position of the interface is calculated explicitly, and a deforming mesh is used in accordance with the interface. On the other hand, front capturing methods are much more robust but they need high mesh resolution. In these methods an auxiliary function is used to identify each component. Volume of fluid methods (VOF) [3], phase field methods and level set methods [4-5] are examples of interface capturing methods. VOF methods are based on conservation laws, so they have excellent conservation properties, but encounter difficulties dealing with large topological changes and geometrical complexities. Level set methods are not as strong as VOF methods in conservation properties, but they are very robust in modeling sophisticated interfaces and rapid changes in topology such as breaking down or coalescence that cannot be handled by a standard front tracking method. The reader is referred for more information to a wide literature and, in particular, the books of Sethian [4] and Osher [6] that give a very clear introduction to these methods.

Sussman and Fatemi [7] developed efficient techniques for simulation of such problems employing level set methods. Similar algorithms have been suggested by others [8-9], but in these methods velocity field is calculated by solving incompressible Navier-Stokes equations that has its own problems inherent while solving second-order nonlinear PDEs. Besides, these two PDEs must be solved simultaneously.

In the last 15 years the Lattice Boltzmann method (LBM) has been used and developed for solving many fluid dynamic problems. LBM is developed from lattice gas automata (LGA) and is a kinetic-based approach. In contrast to the Navier-Stokes solvers that need to treat the nonlinear convective term, LBM solvers avoid the nonlinear convective term, because the convection becomes a simple advection term [10]. Imposing boundary conditions, especially those involving complex geometries, is simpler in LBM. Since the Boltzmann equation is kinetic-based, it can be easily and successfully used for simulation of micro and nano-scale fluids. For more information on the advantages and details of LBM we refer the reader to the comprehensive paper of Yu et al. [10] on the subject.

In present work we have used the method of Sussman and Fatemi [7], but we have replaced conservation laws with the LBM in order to solve the velocities of the domain. The LBM adopted is the single-relaxation-time (SRT) model known as Bhatnagar-Gross-Krook (BGK) model [11]. The proposed algorithm makes use of the advantages of both LBM and level set method.

2 Governing equations

The governing equations controlling the motion of multiphase flows are level set equations and Lattice Boltzmann equation. The velocity field is solved using LBM (BGK).

The calculated velocities are the input of level set method which determines the new position of interface in the velocity field. The level set equation used is similar to convection equation.

$$\frac{\partial \phi}{\partial t} + U.\nabla \phi = 0 \tag{1}$$

2.1 Lattice Boltzmann method

In LBM the velocity of the domain is calculated employing the following differential equation:

$$\frac{\partial f}{\partial t} + \xi.\nabla f = -\frac{1}{\lambda}(f - f^{(eq)}) + \frac{1}{N_\alpha e^2} e_{\alpha i} F_i(x,t) \tag{2}$$

Where $f(x,\xi,t)$ is particle velocity distribution function; $f^{(eq)}$ is equilibrium distribution function (Maxwell-Boltzmann distribution function); F_i is the component of force in i; $e = \Delta x / \Delta t$; λ is the relaxation time; e_α is the velocity vector of the particle in the α direction; N_α is a constant, which is decided by the lattice pattern.

In order to solve for f, Eq. (2) is first discretized in the velocity space using a finite set of velocity vectors $\{\xi_\alpha\}$. In present work the 2-D 9-velocity (2DQ9) single-relaxation-time (SRT) BGK model is used [11]. In 2D9Q model the finite set of velocity vectors consists of nine e_α vectors, which is shown in Fig. 1.

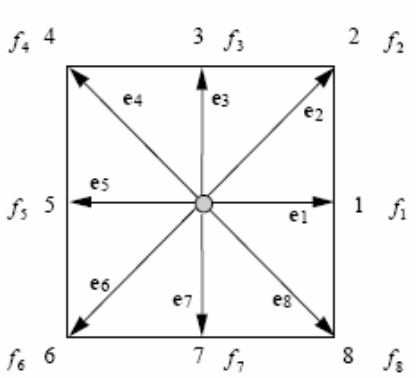


Fig. 1)2-D 9-velocity model

The equilibrium distribution used in D2Q9 model is approximated by a polynomial of macroscopic properties and is derived from conservation laws.

The spatial and temporal discretization of Eq. (2) by an explicit finite difference method yields the lattice Boltzmann equation (Eq. (3)):

$$f_\alpha(x_i + e_\alpha \delta t, t+\delta t) - f_\alpha(x_i,t) = -\frac{1}{\tau}\left[f_\alpha(x_i,t) - f_\varepsilon^{(eq)}(x_i,t)\right] + \frac{\Delta t}{6e^2} e_{\alpha i} F_{\alpha i} \quad (3)$$

where $\tau = \lambda / \Delta t$. The kinematic viscosity of the fluid can be obtained from $\nu = (\tau - 1/2) c_s^2 \delta t$, where C_s is the speed of sound in lattice.

Navier-Stokes and continuity equations can be recovered from lattice Boltzmann equation using Chapmann-Enskog expansion [12].

In low Mach flows that $|u|/c_s << 1$ lattice Boltzmann equation is first-order accurate for macroscopic continuity and momentum equations and can be extended up to second-order accuracy by using a suitable form for force term [13].

2.2 Level set method

Level set methods (LSM) are used to capture the interface. Instead of tracking the interface and dealing with the complex geometry of interface we capture the interface implicitly using an auxiliary scalar function. This makes it possible to simulate great topological changes such as coalescence and breaking-up easily. The level set function is typically a smooth (Lipschitz continuous) function, denoted here as $\phi(x,t)$. The sign of the level set function determines the phase we are dealing with. In our algorithm, the interface is the zero level set of ϕ,

$$\Gamma = \{x \mid \phi(x,t) = 0\}. \quad (3)$$

Without loss of generality assume $\phi < 0$ in low density region (gas) and $\phi > 0$ in high density region (liquid), therefore we have

$$\phi(x,t) = \begin{cases} > 0, & x \in liquid \\ = 0, & x \in \Gamma \\ < 0, & x \in gas \end{cases}. \quad (4)$$

The properties of the fluid, such as density and viscosity, are functions of $\phi(x,t)$.

$$\rho(\phi) = \rho_1 H(\phi) + \rho_2 (1 - H(\phi)) \quad (5)$$

and similarly,

$$\mu(\phi) = \mu_1 H(\phi) + \mu_2 (1 - H(\phi)) \quad (6)$$

that $H(\phi)$ is the Heaviside function given by

$$H(\phi) = \begin{cases} 0, & \phi < 0 \\ \frac{1}{2}, & \phi = 0 \\ 1, & \phi > 0 \end{cases}. \quad (7)$$

When the level set function is a smooth distance function, the interface will have a constant thickness. The unit normal of the interface, from gas into liquid, and the curvature of it can easily be expressed in terms of $\phi(x,t)$ such as:

$$n = \left.\frac{\nabla\phi}{|\nabla\phi|}\right|_{\phi=0} \text{ and } \kappa = \nabla.\left.\left(\frac{\nabla\phi}{|\nabla\phi|}\right)\right|_{\phi=0}. \quad (8)$$

Since the interface moves with the velocity of the fluid, the evolution of ϕ is governed by convection equation,

$$\frac{\partial\phi}{\partial t} + u.\nabla\phi = 0. \quad (9)$$

2.2.1 Thickness of the interface

If we use Heaviside function as described in Eq. (7), the thickness of the interface will be assumed zero and we will get poor results. Besides, we will face difficulties in using exact Dirac delta function for modeling surface tension. In order to alleviate these problems we will give the interface a thickness of $\varepsilon = \alpha \Delta x$, where $\alpha > 1$. We substitute a smoothed Heaviside function $H_\varepsilon(\phi)$ for the sharp Heaviside function $H(\phi)$. The smoothed Heaviside function $H_\varepsilon(\phi)$ defined as below:

$$H_\varepsilon(\phi) = \begin{cases} 0, & \phi < -\varepsilon \\ \frac{1}{2}\left[1 + \frac{\phi}{\varepsilon} + \frac{1}{\pi}\sin\left(\frac{\pi\phi}{\varepsilon}\right)\right], & |\phi| \le \varepsilon \\ 1, & \phi > \varepsilon \end{cases} \quad (10)$$

and the smoothed delta function is

$$\delta_\varepsilon(\phi) = \frac{dH_\varepsilon(\phi)}{d\phi} \quad (11)$$

and consequently, the thickness of the interface is equal to

$$\frac{2\varepsilon}{|\nabla\phi|}. \quad (12)$$

In the present work the interface must have a constant thickness so that $|\nabla\phi|$ becomes constant near the interface. Level set function must be a signed distance function and present the shortest normal distance to the interface, Γ. A signed distance function has the following properties:

$$|\nabla d| = 1 \quad for \ |\phi| \le \varepsilon, \quad d = 0 \quad for \ x \in \Gamma. \quad (13)$$

As the interface evolves, ϕ will generally drift away from its initialized value as signed distance, thus the technique presented needs to be applied periodically in order to keep ϕ approximately equal to signed distance, the process is called re-initialization. In [5] Sussman, Smereka and Osher proposed a differential equation for the process as

$$\frac{\partial d}{\partial \tau^d} = S(\phi)(1-|\nabla d|), \quad (14)$$

where $S(\phi)$ is

$$S(\phi) = \begin{cases} -1, & \phi < 0 \\ 0, & \phi = 0 \\ 1, & \phi > 0 \end{cases}, \quad (15)$$

$d(x,0) = \phi(x,t)$ and τ^d is fictitious time. Eq. (14) must be solved to reach steady state condition. When the convergence occurs the right hand side will be zero, so $|\nabla d|$ will be equal to zero. Instead of sharp sign function some forms of smooth sign function may be used as

$$S_\varepsilon(\phi) = 2(H_\varepsilon(\phi) - \frac{1}{2}). \quad (16)$$

In order to analyze Eq. (14), we may rewrite it as

$$\frac{\partial d}{\partial \tau^d} + w.\nabla d = S(\phi), \quad (17)$$

where

$$w = S(\phi)\frac{\nabla d}{|\nabla d|}. \quad (18)$$

In the present work the explicit method developed by Sussman and Fatemi [7] is used and the interested reader is referred to the literature for more details on the method.

2.2.2 Surface tension modeling

In many fluid mechanic problems surface tension forces become of utmost importance. In the present work the macroscopic approach suggested by Brackbill et al. [14] has been used and surface tension is modeled as a body force in the vicinity of interface. Similar methods have been proposed by Unverdi and Tryggvason [15], and Chang et al. [16] that also represent surface tension as a body force. The magnitude of the force is proportional to the curvature of the interface $\kappa(\phi)$ and is calculated solving the following relation:

$$\begin{aligned} F_{s.tension} &= -\sigma\kappa(\phi)\nabla H_\varepsilon(\phi) \\ &= -\sigma\kappa(\phi)\delta_\varepsilon(\phi)\nabla\phi \end{aligned}. \quad (19)$$

When the level set function is a signed distance function, the curvature of the interface $\kappa(\phi)$ can be found by solving ϕ from the following relation:

$$\kappa(\phi) = \nabla.\left(\frac{\nabla\phi}{|\nabla\phi|}\right). \quad (20)$$

As mentioned above this force is localized near the interface and is equal to zero far from it.

2.3 The new method (LBLSM)

In the current implementation of level set method the velocities of the domain as the input of level set method must be solved. Sussman and Fatemi [7] used incompressible Navier-Stokes equations for calculating the velocities as below:

$$\begin{aligned} &\rho(\phi)\frac{\partial u}{\partial t} + \rho(\phi)u.\nabla u + \nabla p \\ &-\nabla.(2\mu(\phi)D) = -\sigma\kappa(\phi)\delta(\phi)\nabla\phi \\ &+\rho(\phi)g, \ \nabla u = 0 \end{aligned} \quad (21)$$

where ρ and μ are density and viscosity respectively, δ is the Dirac delta function and D is the rate of deformation tensor. We must use Eq. (21) in all the nodes, so after each time step the velocities will change but the densities will remain the same.
Considering Eq. (21), we see that the left hand side is the single-phase Navier-Stokes equation and the right hand side can be considered as a body force term, so Eq. (21) can be replaced by the lattice Boltzmann equation with a force term. If we implement this algorithm, it is seen that after each time step the densities of the two neighbor nodes, especially those about the interface, affect each other and spurious vortexes form near the interface. This problem intensifies in case of high density ratios. In order to solve this difficulty the following procedure is used. Eq. (21) may be rewritten as

$$\begin{aligned} &\frac{\partial u}{\partial t} + u.\nabla u + \frac{\nabla p}{\rho(\phi)} - \frac{\nabla.(2\mu(\phi)D)}{\rho(\phi)} \\ &= -\frac{\sigma\kappa(\phi)\delta(\phi)\nabla\phi}{\rho(\phi)} + g \end{aligned}. \quad (22)$$

The above equation is similar to the Navier-Stokes equation for a fluid with the virtual density equal to unity and forces equal to the left hand side except for the $\frac{\nabla p}{\rho(\phi)}$ term. When pressure gradient is equal to

zero this term vanishes. In order to avoid this problem we add ∇p and $(\frac{\mu(\phi)}{\rho(\phi)})(\nabla^2 u)$ terms to both sides of the relation and Eq. (22) may be rewritten as

$$\bar{\rho}(\phi)\frac{\partial u}{\partial t} + \bar{\rho}(\phi)u.\nabla u + \nabla p - \bar{\mu}(\phi)(\nabla^2 u) = \bar{F} \quad (23)$$

$$\bar{F} = \frac{\nabla.(2\mu(\phi)D)}{\rho(\phi)} - \bar{\mu}(\phi)(\nabla^2 u) - \frac{\sigma\kappa(\phi)\delta(\phi)\nabla\phi}{\rho(\phi)} + g - \frac{\nabla p}{\rho(\phi)} + \nabla p \quad (24)$$

where $\bar{\rho}(\phi)$ is the virtual density approximately equal to unity; $\bar{\mu}(\phi)$ is the virtual viscosity and is equal to $\mu(\phi)/\rho(\phi)$, and the right hand side can be considered as a force term called $\bar{F}$. When the pressure gradient is identical to zero or known, such as hydrostatic pressure, the velocities may be calculated easily in a completely explicit procedure. Besides, as Eq. (23) is solved in the frame of LBM there is no need to worry about the continuity equation, because the mass conservation is satisfied up to first or second order, depending on the force term modification. In this context the velocities are approximately divergence free. When the velocity field is solved by the present algorithm, it will be used by level set method to update ϕ and find the new position of interface. The interested reader is referred to the paper of Mehravaran and Hannani [17] for more explanation on the method.

3 Numerical method

In this Section it will be shown how the governing equations have been implemented numerically. The method proposed by Sussman and Fatemi [7] for the re-initialization process will be used. They focused on preserving the amount of material in each cell, i.e. preserving the area (volume) in two (three) dimensions.

3.1 Level set equation discretization

The level set equation may be solved by first-order upwind method as

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} + u^n\phi_x^n + v^n\phi_y^n = 0, \quad (25)$$

but it may lead to poor results when simulating geometrically complex phenomena. The first-order accurate upwind scheme can be improved upon by using more accurate approximations for ϕ_x^+ and ϕ_x^-. The velocity u is used to decide whether ϕ_x^+ or ϕ_x^- should be used, but the approximations for spatial derivatives ϕ_x^+ or ϕ_x^- can be improved significantly. The methods used in the present work are known as essentially non oscillatory (ENO) method and weighted essentially non oscillatory (WENO) method. In ENO method we use the smoothest possible polynomial interpolation to find ϕ and then differentiate to obtain ϕ_x, but in WENO method weighted convex approximation of three possible ENO approximations is used (see [6] for more information on ENO and WENO methods).

In Section 2.2 we explained the importance of maintaining level set function ϕ as a signed distance function from the interface. When the level set function updates it will distort and may lose its property of being a signed distance function. Ideally the interface remains stationary during the re-initialization process, but as we solve the re-initialization equation numerically the interface may have a small movement. Sussman and Fatemi [7] proposed an improvement to the standard re-initialization process. Since their application was multiphase incompressible flow, they focused on preserving the amount of material in each cell, i.e. preserving the area (volume) in two (three) dimensions. The interested reader is referred to [7] for more explanation on the details of the volume constrained re-initializing method. The developed constraint will significantly improve the accuracy of solving Eq. (14).

4 Numerical results and discussion

In this part several 2D problems has been solved using the hybrid formulation of lattice Boltzman and level set methods.

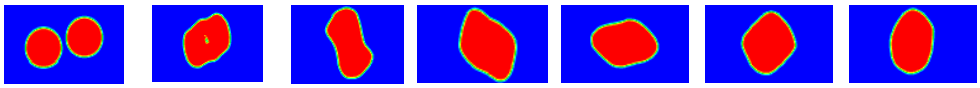
4.1 Binary droplet collision

In this part coalescence of two droplets has been solved; the dimensionless parameters for binary droplet collisions are the Weber number $We = \rho_L D' V^2/\sigma$, the Reynolds number $\mathrm{Re} = \rho_L D' V/\mu_L$ and the impact parameter $Bo = X/D'$, where X is the distance from the center of one droplet to the relative velocity vector placed on the center of the other droplet and D' is the diameter of each droplet. The problem was experimentally studied for water droplets 356 μm in diameter with a Weber number of 70.8, an impact parameter of .25, and a Reynolds number of 327.7 by Qian and Law [18] and is shown in Fig. 2a. In our simulation we imposed periodic boundary conditions on all of the boundaries, there are large differences between the densities and viscosities of the components; $\rho_l/\rho_g = 1000$ and $\mu_l/\mu_g = 100$. The two droplets collide with velocities of $\pm.08$. The mesh used in the simulation is 300×150 and steps

are $\Delta x = \Delta y = \Delta t = .001$. The dimensions used are not exactly those studied by Qian and Law [18], but they are chosen somehow to lead to similar We, Re, and Bo numbers. We use non-dimensional time as $t^* = tV / D$ where V is the relative velocity of two droplets. In our simulation the maximum error in mass (or area) was less than .07, and the average error was less than half of this amount, and is due to the fact that we have solved the problem in the framework of lattice Boltzmann method which satisfies mass and momentum conservation laws simultaneously.

Fig. 2.a)

Fig. 2.b)



$t^* = 0.0$ $t^* = 1.$ $t^* = 3.2$ $t^* = 4.8$ $t^* = 6.4$ $t^* = 8.5$ $t^* = 10.1$

Fig. 2) Time evolution of droplet deformation in non-dimensional time t^* and a comparison between a) experimental photographs [18] and b) the results of numerical simulation for $\mathrm{Re} = 327.7$, $We = 70.8$ and $Bo = .25$.

In spite of the fact that our code is based on a 2D/Cartesian grid and we have neglected pressure gradient, we see that there is good agreement with the experimental results. To get better results we may extend our code to 3D.

In coalescence collision, the momentum of colliding drops is high enough to push out. gas layer entrapped between them, but the entrapment of a small air bubble in high energy impacts is experimentally observed. Mehdi-Nejad et al. [19] reported that air bubble may form under impacting droplet on a solid surface (Fig. 3). Bubble entrapment may also happen in the case of droplet impact on a liquid [20]. This phenomenon is observed in our recent simulation as well (Fig. 4), but the entrapped bubble disappears gradually. When two drops approach each other, air is forced out in the gap between them. Increased air pressure between drops creates a depression in combined drop in which air is trapped [19] and the pressure of the entrapped bubble increases. As we have neglected this pressure gradient in our simulation, the bubble may not persist long and disappears due to diffusion slowly.

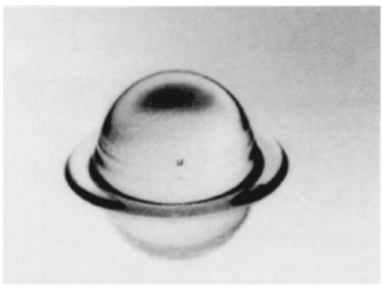
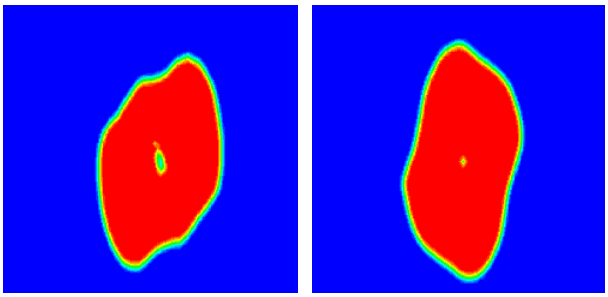


Fig. 3) Impact of N-heptane on a solid surface; air bubble is visible inside the drop [12].



$t^* = 1.$ $t^* = 1.6$

Fig. 4) Entrapment of a small bubble after coalescence using LBLSM.

4.2 Triple droplet collision

We have simulated the behavior of three droplets after collision; the droplets are located on corners of a quadrilateral triangle and the velocities are directed at the angle of 45 degrees towards the horizon, so the problem is only symmetric relative to the horizontal axis. The velocities and geometry of droplets are shown in Fig. 5.

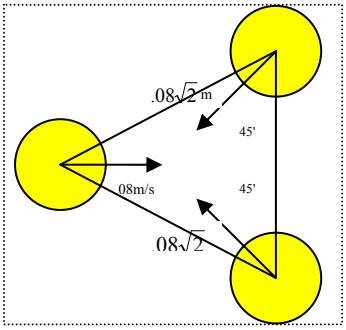


Fig.5) Geometry and velocities of droplets before collision

In our simulation we imposed zero gradient boundary conditions on all of the boundaries, we assume large differences between the densities and viscosities of the

components; $\rho_l / \rho_g = 1000$ and $\mu_l / \mu_g = 100$. The mesh used in the simulation is 200×200 and steps are $\Delta x = \Delta y = \Delta t = .001$. We use the velocity of the left hand side droplet (V=.08 m/s) for calculating We and Re numbers, that will lead to dimensionless parameters of $We = 17.7$ and $\mathrm{Re} = 164$. The maximum error in mass (or area) was about .04. The simulation is shown in Fig. 6.

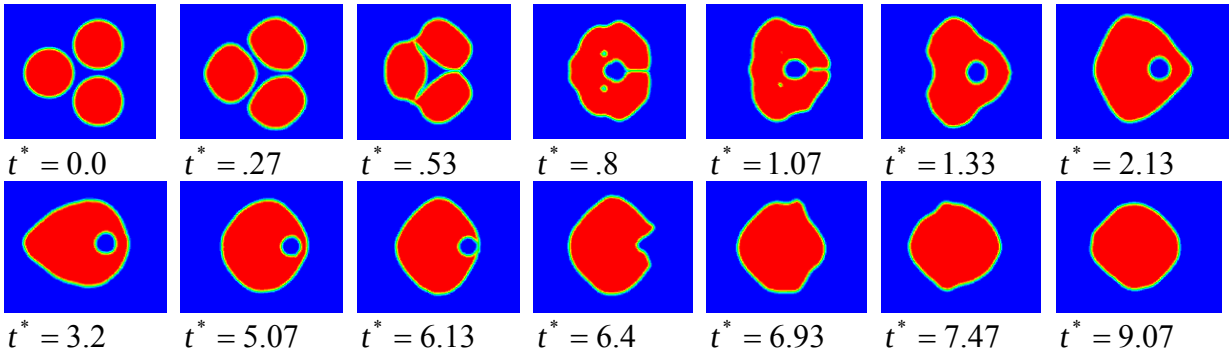


Fig. 6) Time evolution of droplet deformation in non-dimensional time $t^* = tV / D'$ according to the results of numerical simulation for $\mathrm{Re} = 164$ and $We = 17.7$.

5 Concluding remarks

A hybrid lattice Boltzmann level set method (LBLSM) for incompressible two-phase immiscible fluids with large density differences has been developed. The method can simulate two-phase flows with density ratio up to 1000 and viscosity ratio up to 100, especially in case of zero or known pressure gradient. The coalescence of two and three droplets after collision has been simulated by the current method. The simulations compare well with experimental or analytical results. The method is convenient for capturing complex geometries.

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