Numerical Study of Bubble Coalescence by Multiphase MPS Method

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Abstract

In present study, a new mesh-less multiphase method is developed based on the IMPS (Improved Moving Particle Semi-implicit) method and applied to simulate bubble coalescence. In this method, the multiphase system is treated as a multi-density and multi-viscosity system and special interface treatments are introduced for interface region. The new multiphase MPS method is validated through comparisons with data in open literature. In particular, the multiphase MPS method is verified against Hysing et al.'s quantitative benchmark computations of two-dimensional bubble dynamics. Good agreements achieved for the benchmark quantities, including center of mass, and mean rise velocity, which demonstrate the accuracy and stability of the present multiphase MPS method. Then, a numerical study of the coalescence of bubble pairs is conducted and comparison between MPS and experimental results is made. In general, good agreement can be achieved.

Keywords: **Multiphase; MPS; bubble coalescence; CFD**

Introduction

In fluid dynamics, bubbly flow is one of the most important issues and can be found in various natural and industrial processes such as chemical reactors, petroleum refining and boiling. The rising of bubbles in a viscous liquid due to buoyancy is one of fundamental bubbly flow. And when the distances between bubbles become close enough during rising process, interactions of bubbles occur and coalescence may be observed, which can greatly affect the bubble dynamics. Therefore, in order to obtain sufficient acknowledge of the bubble dynamics, the coalescence of bubbles should be primarily investigated.

In recent decades, there have been many experimental and theoretical researches on the coalescence of bubbles [1]-[6]. However, both experimental and theoretical approaches have their limitations. On the one hand, only a small part of flow information can be obtained due to the difficulties in experiments, which results in a limited understanding on coalescence of bubbles. On the other hand, theoretical analysis is also not competitive, because approximate theoretical solutions can be derived only in the cases of small bubble deformations. Therefore, numerical simulations seem to be an effective alternative approach for the study of coalescence of bubbles [7]-[10], with the development of computer technology and computational fluid dynamics (CFD) in recent years. However, the numerical study of bubble coalescence is challenging due to the tracing of largely deformation of multiphase interface. For traditional numerical methods which are based on meshes or grids, there is difficulty in the maintenance of sharp or fragmented interfaces and the meshes containing the interface

need extra and complicated treatments. Besides, the numerical diffusion induced by the advection term is also an unavoidable problem when using these methods.

Through the past few years, the mesh-less particle methods, as a new generation of numerical methods, have been developed energetically and provide a good solution to the problems mentioned above. In the mesh-less particle method, the calculation domain is dispersed by a set of particles with Lagrangian description, which means the profile of interface is automatically presented by the particles distribution, without need of additional capture or tracking procedure. Therefore, particle methods are particularly suitable for problems with large deformation of interface or free surface, like the coalescence of bubbles. Furthermore, numerical diffusion in the discretization of advection term is eliminated because of the use of substantial derivative in governing equations for Lagrangian system. In this paper, the moving particles semi-implicit (MPS) method, which is one of the most commonly known mesh-less particle methods, is employed to simulate the bubble coalescence. Since its being put forward, the MPS method has been successfully applied in a wide range of hydraulic engineering problems, including liquid sloshing [11][12], dam breaks [13][14], water entry [15], and fluid-structure interaction [16]. However, the original MPS method considered only the problems with a single fluid and is not applicable to multiphase flows [17].

A number of significant numerical works have been devoted to extend the MPS method to multiphase flows. The first MPS multiphase method is proposed for solid-liquid two-phase flows [18]. After that, a hybrid MPS-FVM method is developed for the viscous, incompressible, multiphase flows, in which the heavier fluid is represented by moving particles while the lighter fluid is defined on the mesh [19]. Shakibaeinia and Jin [20] studied the multiphase flows by treating the multiphase system as a multi-viscosity and multi-density system, but the unphysical penetration is observed due to the less consideration of interface tension force. Khayyer and Gotoh [21] derived a first-order density smoothing scheme for multiphase flows characterized by high density ratios, and successfully applied this scheme to various multiphase problems including bubble rising. Two multiphase MPS methods, the MMPS-HD and MMPS-CA method are developed by Duan et al. [22]. In MMPS-HD method, harmonic mean density is utilized to avoid extremely large acceleration at interface. In MMPS-CA method, new stable formulations are developed to keep acceleration continuous at interface. Chen et al. [23] preformed a two-dimensional numerical simulation of the motion and coalescence of bubble pairs rising in the stationary liquid pool, in which the single-phase MPS method is utilized and the bubble region is simply regarded as a vacuum.

In present study, a multiphase method is developed based on the IMPS method and special treatments on the two-phase interface. In our method, the multiphase system is treated as the multi-density and multi-viscosity fluid. The interparticle viscosity defined by the harmonic mean viscosity of two particles is firstly adopted to consider the interaction between different phases. Then the density smoothing technique is employed to reduce pressure discontinuity crossing the interface and obtain the continuous acceleration and velocity fields. The influence of surface tension force on the interface is considered through a contoured continuum surface force (CCSF) model. The present multiphase MPS is then verified against Hysing et al.'s quantitative benchmark computations of two-dimensional bubble dynamics [24]. Good agreements are achieved for the benchmark quantities, including center of mass, and mean rise velocity, which demonstrates the accuracy and stability of the present multiphase MPS method. Finally, a numerical study of the coalescence of bubble pairs is conducted and comparison between MPS and experimental results is made. In general, good agreement can be achieved.

Numerical Methods

Improved MPS Method

Due to less accurate formulations, the original MPS method suffered from some non-physical fluid motions and pressure oscillations. In this paper, we employed an improved MPS method, which includes improved schemes. In IMPS method, the governing equations for incompressible viscous fluid in Lagrangian system are employed, which can be expressed by continuity and momentum equations:

$$\frac{D\rho}{Dt} = -\rho\left(\nabla \cdot \boldsymbol{V}\right) = 0 \tag{1}$$

$$\rho\frac{D\boldsymbol{V}}{Dt} = -\nabla P + \mu\nabla^2\boldsymbol{V} + \mathbf{f} \tag{2}$$

where $\boldsymbol{V}$, t, ρ, P, μ and $\mathbf{f}$ represent the velocity vector, time, fluid density, pressure, dynamic viscosity and the body force, respectively. Similar with the solving strategy adopted by Shakibaeinia and Jin [20] and Duan et al. [22], in present method, the governing equations for all fluids belonging to liquid or bubble are uniform and solved together, thus the multiphase system is treated as a single fluid with multi-density and multi-viscosity.

In particle method, a particle interacts with its neighboring particles covered with kernel function $W(r)$. In present study, the kernel function without singularity is employed [25].

$$W(r) = \begin{cases} \dfrac{r_e}{0.85r + 0.15r_e} - 1 & 0 \le r < r_e \\ 0 & r_e \le r \end{cases} \tag{3}$$

where r is distance between particles and r_e is the effect radius.

In MPS method, all terms of differential operators on the right hand of governing equations are replaced by particle interaction models, including the gradient, divergence and Laplacian model, defined as

$$<\nabla\phi>_i = \frac{D}{n^0}\sum_{j\neq i}\frac{\phi_j - \phi_i}{|\boldsymbol{r}_j - \boldsymbol{r}_i|^2}(\boldsymbol{r}_j - \boldsymbol{r}_i)\cdot W(|\boldsymbol{r}_j - \boldsymbol{r}_i|) \tag{4}$$

$$<\nabla\cdot\boldsymbol{\Phi}>_i = \frac{D}{n^0}\sum_{j\neq i}\frac{\left(\boldsymbol{\Phi}_j - \boldsymbol{\Phi}_i\right)\cdot\left(\boldsymbol{r}_j - \boldsymbol{r}_i\right)}{|\boldsymbol{r}_j - \boldsymbol{r}_i|^2}W(|\boldsymbol{r}_j - \boldsymbol{r}_i|) \tag{5}$$

$$<\nabla^2\phi>_i = \frac{2D}{n^0\lambda}\sum_{j\neq i}(\phi_j - \phi_i)\cdot W(|\boldsymbol{r}_j - \boldsymbol{r}_i|) \tag{6}$$

where ϕ is an arbitrary scalar function, $\boldsymbol{\Phi}$ is an arbitrary vector, D is the number of space dimensions, n^0 is the particle number density at initial arrangement, λ is a parameter defined as

$$\lambda = \frac{\sum_{j\neq i}W(|\boldsymbol{r}_j - \boldsymbol{r}_i|)\cdot|\boldsymbol{r}_j - \boldsymbol{r}_i|^2}{\sum_{j\neq i}W(|\boldsymbol{r}_j - \boldsymbol{r}_i|)} \tag{7}$$

which is applied to keep the variance increase equal to that of the analytical solution.

In case of pressure gradient model, direct application of Eq. (4) may bring about the problem of tensile instability. In this paper, we employed the modified pressure gradient model [26], written as:

$$< \nabla P >_i = \frac{D}{n^0} \sum_{j \neq i} \frac{P_j - P_{i\_\min}}{| \boldsymbol{r}_j - \boldsymbol{r}_i |^2} (\boldsymbol{r}_j - \boldsymbol{r}_i) \cdot W(| \boldsymbol{r}_j - \boldsymbol{r}_i |) \tag{8}$$

where $P_{i\_\min}$ represents the minimal pressure among neighboring particles of particle *i*.

Fluid density in MPS method is represented by particle number density. Therefore, the incompressible condition can be satisfied by keeping the particle number density constant. For this purpose, each time step in MPS method is divided into two stages: In the first stage, temporal velocity of particles is obtained using viscous and body forces terms, which can be explicitly calculated. In the second stage, pressure term is implicitly calculated by solving the Pressure Poisson Equation (PPE), and the velocity and position of particles are updated to make the fluid incompressible. The PPE in present MPS solver is defined as

$$< \nabla^2 P^{n+1} >_i = (1-\gamma) \frac{\rho}{\Delta t} \nabla \cdot \boldsymbol{V}_i^* - \gamma \frac{\rho}{\Delta t^2} \frac{< n^* >_i - n^0}{n^0} \tag{9}$$

where γ is a blending parameter with a value less than 1. The range of $0.01 \leq \gamma \leq 0.05$ is recommended according to the numerical tests conducted by Lee et al. [27]. In this paper, $\gamma = 0.01$ is adopted for all simulations.

The kinematic and dynamic free surface boundary conditions should be imposed on the free surface particles. The kinematic boundary condition is automatically satisfied in Lagrangian method, while the dynamic free surface boundary condition is implemented by setting zero pressure on the free surface particles. To impose the dynamic free surface boundary condition, free surface particles should be detected at first. In present method, a function [25] based on the asymmetric arrangement of neighboring particles of the center particle is defined as:

$$< \boldsymbol{F} >_i = \frac{D}{n^0} \sum_{j \neq i} \frac{1}{| \boldsymbol{r}_i - \boldsymbol{r}_j |} (\boldsymbol{r}_i - \boldsymbol{r}_j) W(\boldsymbol{r}_{ij}) \tag{10}$$

where the vector function $\boldsymbol{F}$ represents the asymmetry of arrangements of neighbor particles. Particles satisfying

$$< | \boldsymbol{F} | >_i \ > \ 0.9 | \boldsymbol{F} |^0 \tag{11}$$

are judged as free surface particles, where $|\boldsymbol{F}|^0$ is the value of $|\boldsymbol{F}|$ for surface particles at initial arrangement.

Special Treatments for Multi-phase Flows

To extend the IMPS method into multiphase flows, special treatments are introduced in present paper. For multiphase flows, the mathematical discontinuity of density at two-phase interface causes a discontinuous acceleration field and accordingly numerical instabilities. In present study, the density smoothing scheme [20][21] is adopted for interface particles, which is based on a simple spatial averaging as follow:

$$< \rho >_i = \frac{\sum_{j \in I} \rho_j W(r_{ij}, r_e)}{\sum_{j \in I} W(r_{ij}, r_e)} \tag{14}$$

where I include particles i and all its neighboring particles.

In present paper, the multi-viscosity model [20] is employed to deal with viscosity discontinuity cross interface. With the multi-viscosity model, the viscous term in Eq. (2) can be presented as:

$$< \mu \nabla^2 \boldsymbol{V} >_i = \frac{2D}{\lambda n^0} \sum_{j \neq i} \mu_{ij} (\boldsymbol{V}_j - \boldsymbol{V}_i) W(| \boldsymbol{r}_j - \boldsymbol{r}_i |) \tag{15}$$

$$\mu_{ij} = \frac{2\mu_j \mu_i}{\mu_j + \mu_i} \tag{16}$$

where μ_{ij} represents the interparticle viscosity between particles i and j. It is obvious that μ_{ij} is equal to the real viscosity of one fluid ($\mu_{ij}=\mu_i=\mu_i$) when particles i and j belong to a same phase.

For multiphase flows, interface tension effects are important when deformations of fluid interfaces are involved. One of the most widely used approach for incorporation of interface tension effects is the continuum surface force (CSF) method [28]. In this approach, surface/interface tension is converted into a body force in a transition region across the interface. Therefore, for particles in this transition region, the momentum equation Eq. (2) of governing equations transforms into

$$\rho \frac{D\boldsymbol{V}}{Dt} = -\nabla P + \mu \nabla^2 \mathbf{V} + \mathbf{f} + \mathbf{f}_s \tag{17}$$

$$\mathbf{f}_s = \sigma \kappa \nabla C \tag{18}$$

where $\mathbf{f}_s$ is the interface tension, σ is the surface tension coefficient, κ is the interface curvature, C is a color function defined as:

$$C_i = \begin{cases} 0 & \text{particle } i \text{ belongs to the specified phase} \\ 1 & \text{particle } i \text{ belongs to the other phase} \end{cases} \tag{19}$$

The surface tension coefficient σ is known for a certain fluid. Therefore, the most important issue in CSF model is the calculation of interface curvature κ, which is also the most difficult issue. In present study, the curvature is analytically calculated based on the contour of color function [29]. The contour of color function C is approximately regarded as the profile of interface. With the contour of color function obtained, the interface curvature can be calculated. The calculation process of curvature can be simply divided into four steps. First, the value of the color function f at an arbitrary location (x, y) in the vicinity of the target particle i can be obtained by performing a spatial weighted averaging of all the neighboring particles of particle i, through the implementation of a Gaussian kernel function G:

$$f(x, y) = \frac{\sum_j C_j G(\left|\boldsymbol{r} - \boldsymbol{r}_j\right|, r_s)}{\sum_j G(\left|\boldsymbol{r} - \boldsymbol{r}_j\right|, r_s)} \tag{20}$$

$$G(r_{ij}, r_s) = \frac{9}{\pi r_s^2} \exp\left(-\frac{9 r_{ij}^2}{r_s^2} \right) \tag{21}$$

where r_s represents the effect radius of the Gaussian kernel function.

Second, $f(x, y)$ is expanded at point i through the Taylor series expansion:

$$\begin{aligned} f(x,y) = f(x_i, y_i) + f_{x,i}(x - x_i) + f_{y,i}(y - y_i) + \frac{1}{2} f_{xx,i}(x - x_i)^2 \\ + f_{xy,i}(x - x_i)(y - y_i) + \frac{1}{2} f_{yy,i}(y - y_i)^2 + O(r_s^3) \end{aligned} \tag{22}$$

where the subscripts x and y represent the partial derivatives with respect to x and y at particle i, respectively. The calculation of the partial derivatives can be found in [29]. $O(r_s^3)$ is the high order error term which has no influence on the accuracy of curvature calculation and can be omitted [29].

Third, considering that the local contour of color function passing through particle i must satisfy $f(x, y) = f(x_i, y_i)$, we can obtain the equation of the local contour at particle i from Eq. (22):

$$f_{x,i}(x - x_i) + f_{y,i}(y - y_i) + \frac{1}{2} f_{xx,i}(x - x_i)^2 + f_{xy,i}(x - x_i)(y - y_i) + \frac{1}{2} f_{yy,i}(y - y_i)^2 = 0 \tag{23}$$

Finally, the curvature at particle i can be analytically calculated as follow:

$$\kappa_i = \frac{y''}{\left(1 + y_i'\right)^{3/2}} = \frac{2 f_{x,i} f_{y,i} f_{xy,i} - f_{x,i}^2 f_{yy,i} - f_{y,i}^2 f_{xx,i}}{\left(f_{x,i}^2 + f_{y,i}^2 \right)^{3/2}} \tag{24}$$

Numerical Validation

The new multiphase method is verified against Hysing et al.'s quantitative benchmark computations of two-dimensional bubble rising [24]. The initial condition and parameters for the test case are shown in Fig. 1 and Table 1. On the one hand, the qualitative results of the bubble shapes during rising process are compared. On the other hand, some quantitative comparisons are also provided, including the center of mass (y_{bubble}) and rise velocity of the bubble (u_{bubble}), which are defined as below:

$$y_{\text{bubble}} = \left(\sum_i^{N_{\text{bubble}}} y_i \right) / N_{\text{bubble}} \tag{25}$$

$$u_{\text{bubble}} = \left(\sum_i^{N_{\text{bubble}}} u_{yi} \right) / N_{\text{bubble}} \tag{26}$$

Where N_{bubble} is the total number of bubble particles, y_i is the vertical coordinate of the bubble particle i, u_{yi} is the vertical velocity of the bubble particle i.

Table 1. Parameters for the simulation of bubble rising

Parameters	Value	Unit
Computational domain	1×2	m
Particle spacing	0.01	m
Total particle number	25389	/
Bubble diameter (r_0)	0.5	m
Liquid density	1000	kg/m^3
Bubble density	100	kg/m^3
Liquid viscosity	10	kg/(m. s)
Bubble viscosity	1	kg/(m. s)
Time step size	0.0001	s
Gravitational acceleration	-0.98	s/m^2

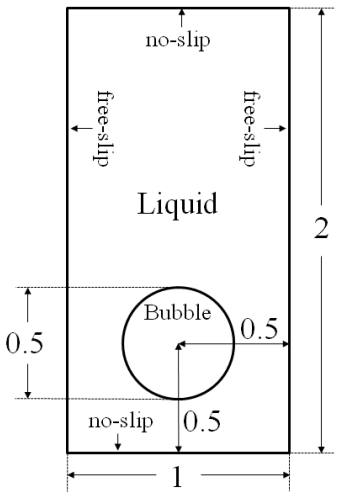


Figure 1. Initial condition for the validation case

In present case, the non-dimensional *Bo* number can be defined as

$$Bo = \frac{\rho_1 U_g^2 L}{\sigma} \tag{27}$$

where ρ_1 refers to the density surrounding heavier fluid, $L=2r_0$ is the characteristic length scale, $U_g^2=g2r_0$ is the gravitational velocity. The *Bo* number is relatively small in this case, equal to 10, which means the surface tension effects are strong enough compared with gravitational forces and can hold the bubble together. As shown in Fig. 2, the rising bubble ends up in the ellipsoidal regime without break up. The bubble shapes simulated by present method at t = 3 s are compared with the benchmarks results, where good agreement are obtained. Furthermore, the results of the evolution of center of mass and rise velocity are presented in Fig. 4. The bubble rises at a growing speed at the early stage, until a largest velocity appears. After that, the rising of the bubble gradually slows down and a steady velocity can be finally reached, which can be called terminal velocity. In general, good agreements with benchmark results can be observed. Besides, the fluctuations of the rise velocity in some other particles methods are not found in present results, due to the improved accuracy and stability of the IMPS.

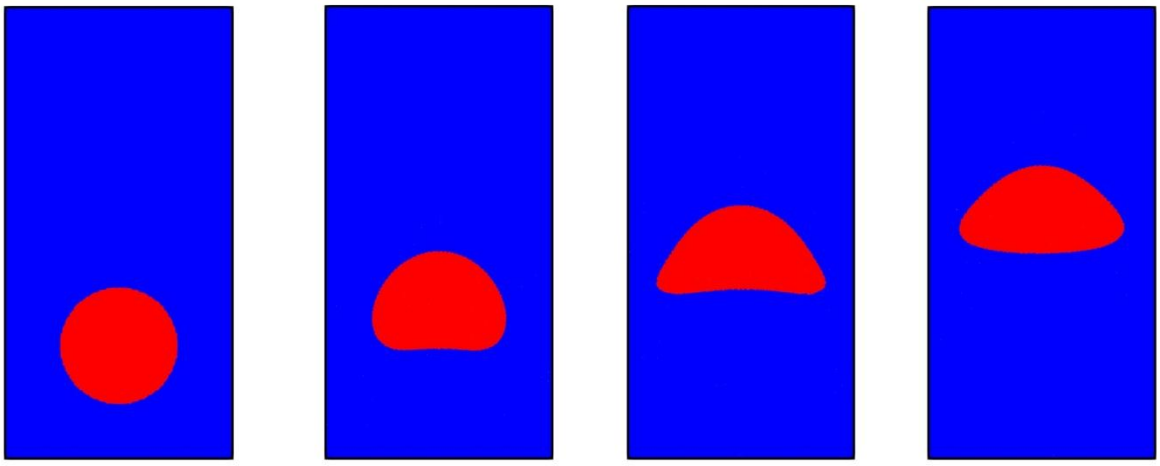


Figure 2: Time evolution of the bubble shapes during rising process. (t = 0 s, 1 s, 2 s, 3 s)

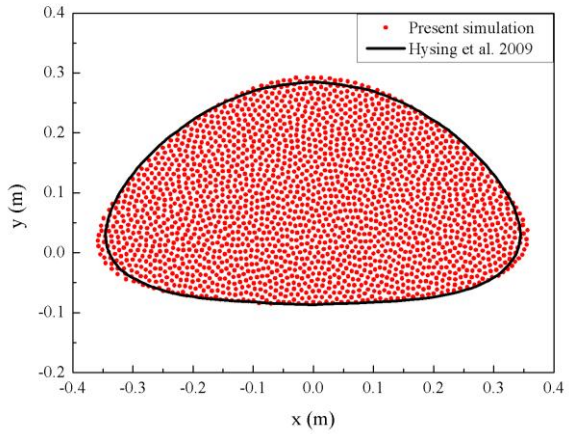


Figure 3: Comparison of bubble shapes at t = 3 s for bubble rising

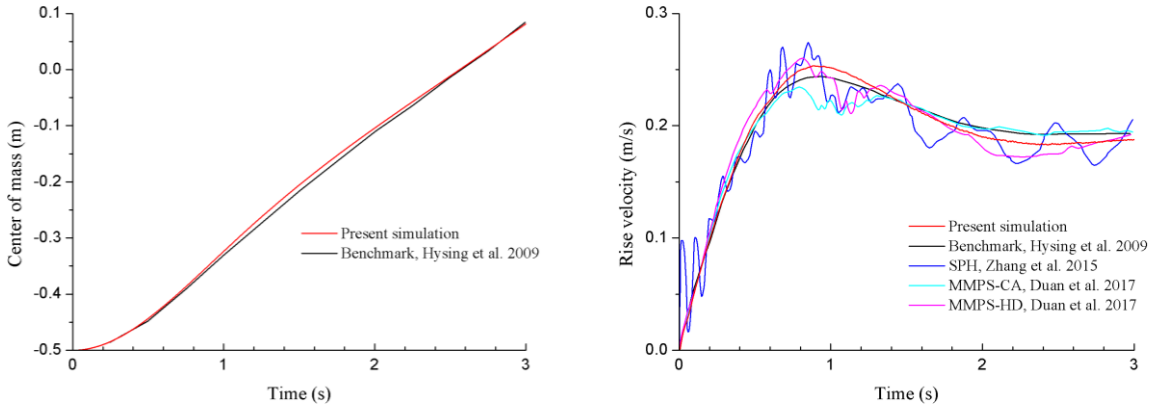


Figure 4: Comparison of center of mass and rise velocity for bubble rising

Numerical Simulation of Bubble Coalescence

In this section, the bubble coalescence is numerically simulated by the newly developed method and comparison between numerical and experimental results is carried out. As shown in Fig. 5, two bubbles are initially arranged side by side at horizontal direction. Then the two bubbles will rise under the effects of buoyancy. According to the Bernoulli's lay, the two bubbles will move closer to each other during the rising process, due to the faster fluid velocity and lower pressure between the two bubbles, and bubble coalescence can occur. The initial condition and parameters for the test case are shown in Fig. 5 and Table 2.

Fig. 6 shows the snapshots of the coalescence of two bubbles obtained by present multiphase MPS method and observed in experiment [2] at some characteristic time instants. It can be seen from Fig. 6 that as the two bubbles rose, they would at first approach and finally get in touch with each other. Then a gas-bridge forms between and connected the two bubbles. Under the effects of interface tension force, the liquid between two bubbles are rapidly excluded and the gas bridge expands in the vertical direction, which results in the coalescence of the two bubbles. It can be clearly seen from comparison between Fig. 6(a) and Fig. 6(b) that the coalescence processes obtained the MPS simulation and experiment shows good accordance in general.

Table 2. Parameters for the bubble coalescence

Parameters	Value	Unit
Computational domain	0.05×0.1	m
Particle spacing	0.00025	m
Total particle number	90489	/
Bubble diameter ($2r_0$)	0.01	m
Liquid density	1000	kg/m^3
Bubble density	10	kg/m^3
Liquid viscosity	1.31×10^{-2}	kg/(m. s)
Bubble viscosity	1.31×10^{-4}	kg/(m. s)
Time step size	0.00000125	s
Gravitational acceleration	9.8	s/m^2

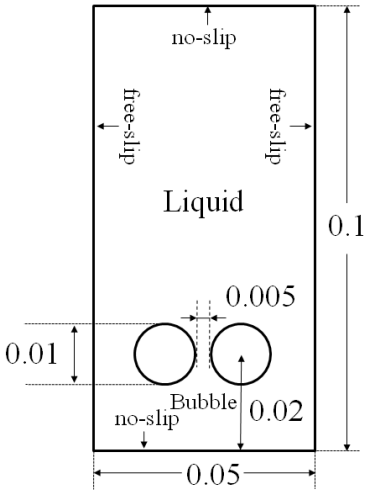
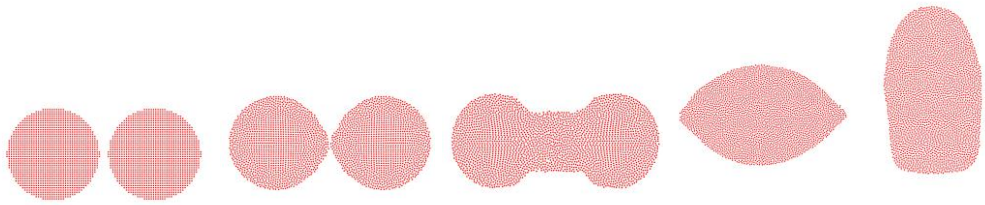
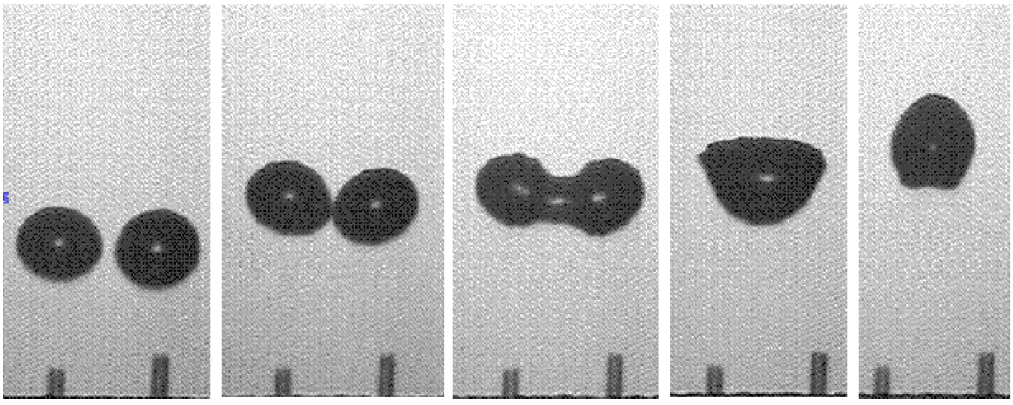


Figure 5. Initial condition for the bubble coalescence



t=0 s *t*=0.02 s *t*=0.04 s *t*=0.09 s *t*=0.025 s

(a)



(b)

Figure 6. Comparison of coalescence of two bubbles between present MPS simulation and experiment in the literature: (a) simulative result; (b) experimental result from literature [2].

Conclusions

In this study, the numerical study of bubble coalescence is carried out by using a newly developed multiphase MPS method based on the IMPS method. The present method treats the multiphase system as the multi-density and multi-viscosity fluid, thus only a single set of equations needs to be solved for all phases. Besides, extra density smoothing technique, interparticle viscosity model and surface tension model are included in the present method for interface particles. The new method is verified against Hysing et al.'s quantitative benchmark computations of two-dimensional bubble dynamics [24]. In general, both the qualitative comparison of bubble shapes and quantitative comparisons of center of mass and mean rise velocity show good agreement, validating the accuracy and stability of the present multiphase MPS method. Then, the newly developed method is applied to simulate bubble coalescence. The coalescence process obtained by present method is in good agreement with the experimental results observed by Duineveld [2].

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