A Filtered Cumulant Lattice Boltzmann Method for Two-phase Flow Simulations

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A novel filtered cumulant lattice Boltzmann method (FCLBM) has been developed to solve advanced two-phase flow problems such as those of violent flows or with complex geometry. The proposed method employs a combination of a velocity-based formulation of the two-phase LBM with a cumulant collision model and a velocity-field filter to obtain time-dependent velocity and pressure fields. For the interface capturing, a conservative phase-field lattice Boltzmann method (CPFLBM) is employed which guarantees the mass conservation. The proposed method has been validated using several benchmark problems and the results show good agreements with the references. The proposed method has been applied to simulate violent two-phase flows and the results show qualitatively good agreements with the references. Currently, the proposed method is being studied for two-phase flow problems with complex geometry.

1. Introduction

LBM has become a popular alternative method in computational fluid dynamics. Due to its simple kinetic equation [1], LBM has several advantages such as no pressure Poisson equation, efficient for massive parallel computation, and capable of handling complex geometries.

Because of its promising features, LBM is continually being extended for a wider range of applications. One such application is the simulation of two-phase flow problems such as Rayleigh-Taylor instability, bubble, and droplet dynamics. Many models were developed to for such applications such as Ba's color-gradient, Wu's pseudo-potential, Huang and Wang's free-energy, Zheng's mean-field, Kim and Pitsch's velocity-formulation, Wang's flux-solver, Fakhari's phase-field, and Inamuro's improved lattice kinetic models [2-9]. All these models were able to simulate problems with high density ratio, typically about 1000.

Despite the many successes, several problems have not been studied such as the simulation of violent two-phase flows and two-phase flow problems with complex boundaries. In case of violent two-phase flows, the problem is difficult to solve because its density ratio and Reynolds number are high (about 1000 and more than 10^5, respectively), and there are rapid and complex topological changes. The simulation of this problem may be unstable if previous LBMs are applied. In case of the phase flow problems with complex boundaries, the problem may be difficult to solve by conventional method as the applied method must guaranteed mass conservation and stability when dealing with complex boundaries. LBM is known to be conservative and capable of handling complex boundaries.

In this paper, we propose a filtered cumulant two-phase LBM with an adaptive filter and show that it is suited to solve the problem. The filtered cumulant LBM is based on Kim and Pitsch's velocity-formulation model which is extended by employing the cumulant collision model [6, 12]. For the inter-face capturing, the conservative phase-field lattice Boltzmann method is employed which guarantees the mass conservation [13].

2. Numerical methods

Filtered cumulant lattice Boltzmann method (filtered CLBM) is employed to simulate the fluid motion. The cumulant LBM solves the following lattice Boltzmann equation:

$$f_{ijk(x+ic\delta t)(y+jc\delta t)(z+kc\Delta t)(t+\delta t)} - f_{ijkxyzt} = \Omega_{ijkxyzt}, \quad (1)$$

where f is the discrete particle distribution function (PDF), Ω is the discrete collision operator, $\mathbf{x} = (x, y, z)$ is the position, and t is the time. In this work, Eq. (1) is solved on the D3Q27 lattice which consists of 27 discrete velocities $\mathbf{e} = (e_x, e_y, e_z)$, where $i = e_x/c$, $j = e_y/c$, $k = e_z/c$, $i, j, k \in \{\bar{1}, 0, 1\}$ (Miller indices with $\bar{1} \equiv -1$ is used), $c = \delta x/\delta t$ is the lattice speed, δx is the lattice spacing, and δt is the lattice time step. The square of the sound speed of this lattice is $c_s^2 = c/3$.

Eq. (1) is solved by splitting it into collision and streaming steps as follows:

$$f^*_{ijkxyzt} = f_{ijkxyzt} + \Omega_{ijkxyzt}, \quad (2)$$

$$f_{(x+ic\delta t)(y+jc\delta t)(z+kc\Delta t)(t+\delta t)} = f^*_{ijkxyzt}, \quad (3)$$

where f^* is the post-collision PDFs. This is an efficient procedure as the collision step in Eq. (2) is evaluated locally and the streaming step in Eq. (3) is simply advecting the distribution functions.

In this paper, the collision step of Eq. (2) is expressed as the multi-relaxation of cumulants as follows:

$$f^*_{ijkxyzt} = c_{\alpha\beta\gamma} - \omega_{\alpha\beta\gamma}\left(c_{\alpha\beta\gamma} - c^{eq}_{\alpha\beta\gamma}\right) = c^*_{\alpha\beta\gamma}, \quad (4)$$

where c denotes cumulants, $\alpha, \beta, \gamma \in \{0,1,2\}$ are the order of the cumulants, and ω is the relaxation rates. The cumulant collision model has good stability for high Reynolds number problems due to statistical independence among cumulants [12]. The cumulants can be obtained from the distribution function using the following equation:

$$c_{\alpha\beta\gamma} = c^{-(\alpha+\beta+\gamma)} \frac{\partial^{\alpha+\beta+\gamma}}{\partial \Xi_x{}^{\alpha} \partial \Xi_y{}^{\beta} \partial \Xi_z{}^{\gamma}} ln\left(\mathcal{L}\left[f(\underline{\xi})\right](\underline{\Xi})\right)\Big|_{\underline{\Xi}=0}, \quad (5)$$

where $\mathcal{L}$ is the Laplace transformation.

The cumulant collision model is employed within a velocity-based formulation of two-phase LBM. In this formulation, the density is set as a constant ($\rho = 1$), which through Chapman-Enskog analysis leads to the following pressure-less momentum equations [14]:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = \nabla \cdot [\nu(\nabla \mathbf{u} + \nabla^{\mathrm{T}} \mathbf{u})], \quad (6)$$

where the kinematic viscosity ν is related to the flowing relaxation rate:

$$\omega_1 = \left(\frac{3\nu\delta t}{\delta_x^2} + \frac{1}{2}\right)^{-1}. \quad (7)$$

The relaxation rates other than ω_1 are set to unity in this study. Eq. (49) is different from the INSE, therefore several terms are added. The following force is added to add the pressure term:

$$\mathbf{F}^p = -\frac{1}{\rho}\nabla p, \quad (8)$$

where $\mathbf{F}^p$ is the pressure force. The viscosity term is also corrected by adding the following force:

$$\mathbf{F}^\nu = -\frac{\nu}{\rho}\nabla\cdot[\rho(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)], \quad (9)$$

where $\mathbf{F}^\nu$ is the additional viscous force. The body force due to gravity is calculated as:

$$\mathbf{F}^b = \rho\mathbf{g}, \quad (10)$$

where $\mathbf{g}$ is the gravity acceleration. The surface force due to surface tension is modelled by the density-scaled continuous surface force model [15]:

$$\mathbf{F}^s = -\frac{2\rho}{(\rho_l + \rho_h)}\sigma(\nabla\cdot\mathbf{n})\nabla\phi, \quad (11)$$

where σ is the surface tension. Finally, the forces are summed:

$$\mathbf{F} = \mathbf{F}^p + \mathbf{F}^\nu + \mathbf{F}^b + \mathbf{F}^s, \quad (12)$$

The pressure is then calculated from the PDFs as follows:

$$p^{n+1} = p^n + \rho^{n+1}c_s^2\left(\sum_\alpha f_\alpha - 1\right). \quad (13)$$

For stability, a second order filter is applied to the pressure field [6]:

$$\bar{p}(\boldsymbol{x}) = \sum_\alpha p(\mathbf{x} + \mathbf{e}_\alpha\delta t). \quad (14)$$

The filtered pressure field $\bar{p}$ is then used in Eq. (51) and the macroscopic velocity is updated semi-implicitly:

$$\mathbf{u}^{n+1} = \sum_\alpha \mathbf{e}_\alpha f_\alpha + \frac{\mathbf{F}\delta t}{2}. \quad (15)$$

This formulation has recovered the INSE with the following pressure equation:

$$\frac{\partial p}{\partial t} + \rho c_s^2\nabla\cdot\boldsymbol{u} = 0. \quad (16)$$

To satisfy the incompressible flow condition, the Mach number should be kept low:

$$Ma = \frac{|\boldsymbol{u}|}{c_s} \ll 1. \quad (17)$$

Hereafter this formulation is referred as the unfiltered CLBM because the velocity field is unfiltered.

To further enhance its stability for violent two-phase flow, the following adaptive filter is applied to the velocity field:

$$\bar{\mathbf{u}}_{i,j,k} = \mathbf{u}_{i,j,k} + \frac{\delta t}{4\delta x^2}\Big(\left|u_{x\,i+\frac{1}{2},j,k}\right| D_{i+\frac{1}{2},j,k} - \left|u_{x\,i-\frac{1}{2},j,k}\right| + \left|u_{y\,i,j+\frac{1}{2},k}\right| D_{i,j+\frac{1}{2},k} - \left|u_{y\,i,j-\frac{1}{2},k}\right| D_{i,j-\frac{1}{2},k} + \left|u_{z\,i,j,k+\frac{1}{2}}\right| D_{i,j,k+\frac{1}{2}} - \left|u_{z\,i,j,k-\frac{1}{2}}\right| D_{i,j,k-\frac{1}{2}}\Big), \quad (18)$$

with

$$D_{i+\frac{1}{2},j,k} = \boldsymbol{u}_{i,j,k} - \boldsymbol{u}_{i-1,j,k} \quad if\ Pe_{i+\frac{1}{2},j,k} \geq 2, \quad (19)$$

$$D_{i+\frac{1}{2},j,k} = 0 \quad if\ Pe_{i+\frac{1}{2},j,k} < 2, \quad (20)$$

$$Pe_{i+\frac{1}{2},j,k} = \left|\frac{u_x}{\nu}\right|_{i+\frac{1}{2},j,k}, \quad (21)$$

where $\mathbf{u} = (u_x, u_y, u_z)$ is the velocity field, $\bar{\mathbf{u}}$ is the filtered velocity field i, j, k are the cell index in x-, y-, z-direction, respectively. This filter adds an artificial viscosity depending on the Peclet number Pe, analogously to the hybrid differencing scheme for advection equation [16]. Hereafter, the cumulant LBM with this filter is referred as filtered CLBM.

To capture the interface dynamics, the following conservative phase-field lattice Boltzmann method (CPFLBM) **Error! Reference source not found.**:

$$h_\alpha(\boldsymbol{x} + \boldsymbol{e}_\alpha\delta t, t + \delta t) - h_\alpha(\boldsymbol{x}, t) = -\frac{1}{\tau_\phi}\left(h_\alpha(\boldsymbol{x}, t) - h_\alpha^{eq}(\boldsymbol{x}, t)\right), \quad (22)$$

where h_α, τ_ϕ, and $\boldsymbol{e}_\alpha$ are the distribution function, the relaxation time for CPFLBM, and the discrete velocity set, respectively. The equilibrium PDFs for CPFLBM is defined as:

$$h_\alpha^{eq} = w_\alpha\left(\phi\left[1 + \frac{\boldsymbol{e}_\alpha\cdot\boldsymbol{u}}{c_s^2}\right] + \frac{M}{W}\left[1 - 4\left(\phi - \frac{1}{2}\right)^2\right]\frac{\boldsymbol{e}_\alpha\cdot\boldsymbol{n}}{c_s^2}\right). \quad (23)$$

The relaxation time for CPFLBM is defined as:

$$\tau_\phi = Mc_s^2 + \frac{1}{2} \quad (24)$$

Finally, the phase-field variable is computed as:

$$\phi = \sum_\alpha h_\alpha \quad (25)$$

3. Results and Discussions

3.1. 2D single bubble rising

To validate the proposed method in simulating two-phase flows with high density ratio and surface tension, 2D single rising bubble problem is considered. The present technique is benchmarked against two Finite Element Method (FEM) solvers: TP2D (FEM with level set for interface tracking) [17] and Abels' model (FEM with Cahn-Hilliard for interface tracking) [18]. The prior one is based on sharp-interface model whereas the later one is based on diffuse-interface model.

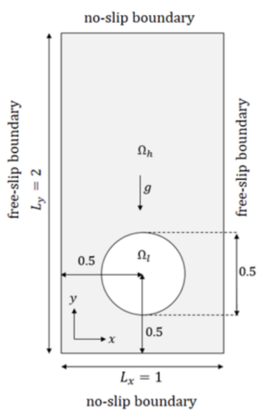

Fig. 1 Schematic of the initial condition of 2D rising bubble

problem.

Fig.1 shows the problem setup, where a bubble of lighter fluid (in Ω_l) is surrounded by a heavier fluid (in Ω_h). As the simulation progresses, the bubble rises and its shape evolves according to the given physical parameters. Two cases were simulated with the physical parameters and dimensionless numbers are shown in Table . The Reynolds number Re and Eotvos number Eo (the ratio of gravitational to surface tension forces) of this problem are calculated as follows:

$$Re = \frac{\rho_h D \sqrt{gD}}{\mu_h}, \tag{26}$$

$$Eo = \frac{\rho_h g D^2}{\sigma}, \tag{27}$$

where D is the bubble's diameter. Case 2 is considered more difficult than Case 1, where more complex bubble shape with thin filaments is expected due to the higher density ratio and Eotvos numbers.

Table 1. Physical parameters and dimensionless numbers in 2D rising bubble problem.

Case	ρ_h	ρ_l	μ_h	μ_l	g	σ	Re	Eo	$\frac{\rho_h}{\rho_l}$	$\frac{\mu_h}{\mu_l}$
1	1000	100	10	1	0.98	24.5	35	10	10	10
2	1000	1	10	0.1	0.98	1.96	35	125	1000	100

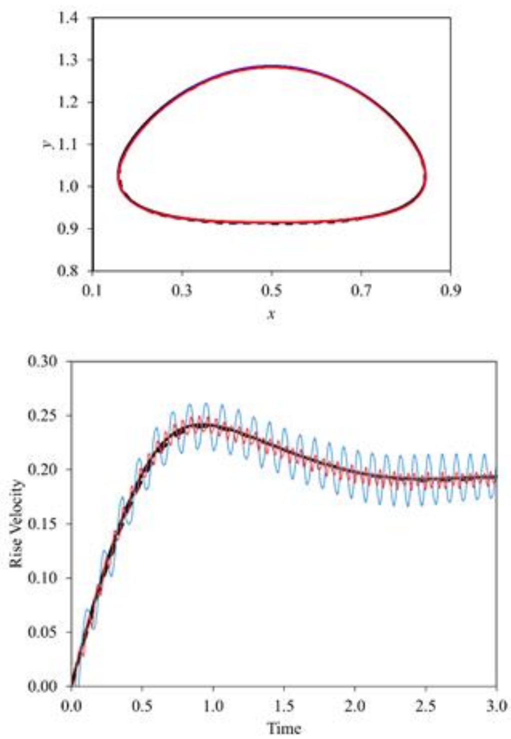

Fig. 2 Bubble shapes at final time (top) and rise velocity (botttom) for Case 1 of the 2D rising bubble problem. Filtered

CLBM with Ma_{max} = 0.007 (red), filtered CLBM with Ma_{max} = 0.014 (blue). References: TP2D (solid black) and Abels (dashed black).

The problem was solved up to the time $T = 3.0$ with mesh resolution $h = 1/320$ and time interval $\Delta t = 1/20000$. The reference TP2D and Abels' models use mesh resolutions $h = 1/320$ and $h = 1/128$, respectively. The mesh depth is set to a single gridpoint with free-slip boundaries. In this setting, both unfiltered and filtered CLBM produces the same result as the Reynolds number is low.

Fig. 2 shows the benchmark results for Case 1. The bubble shapes at the final time from the proposed method agrees very well with the references. Its rise velocity however oscillates about a mean value. This oscillation occurs due to compressibility effects where pressure waves travel with the speed proportional to the sound speed. The oscillation can be reduced by reducing the Mach number. The mean value of the rise velocity however is in good agreement with the references.

Fig. 3 shows the benchmark results for Case 2. The bubble shapes at final time from the proposed method differs from the references, mainly on the bubble's bottom and skirt shape. Better agreement however is obtained with the reference diffuse-interface model (Abels' model). The proposed method belongs to a diffuse-interface model where the interface spans several gridpoints. The difference may be also due to the difference in the calculation of surface tension force: the present algorithm uses the curvature from the phase-field function, whereas TP2D uses a level set function and Abels' model uses a chemical potential model. The decrease of Mach number has a slight effect on the bubble shapes, however it reduces the oscillation of the rise velocity.

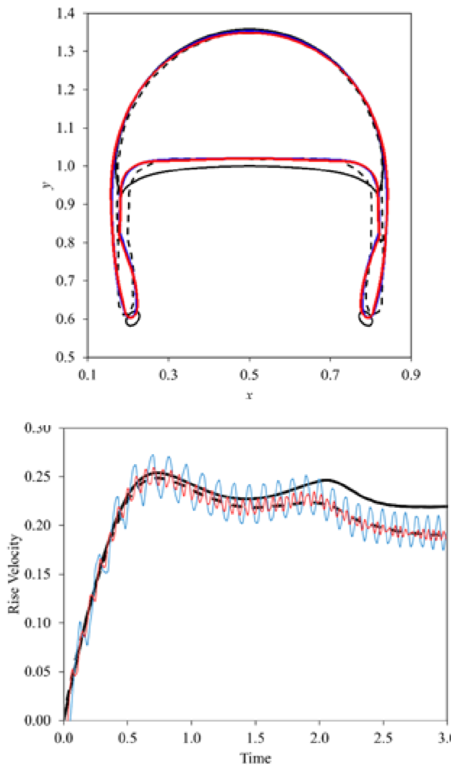

Fig. 3 Bubble shapes at final time (left) and rise velocity (right) for Case 2 of the 2D rising bubble problem. Filtered CLBM with Mamax = 0.012 (red), filtered CLBM with

Mamax = 0.024 (blue). References: TP2D (solid black) and Abels (dashed black).

3.2. 3D dam breaking on a wet floor

In this section, our proposed method is applied to solve a violent two-phase flow, namely the dam breaking on a wet floor problem. The existance of a thin film causes additional complexity in terms of breaking and splashing. To examine its quality, the proposed method is benchmarked against the free-surface LBM by Onodera and Ohashi [19].

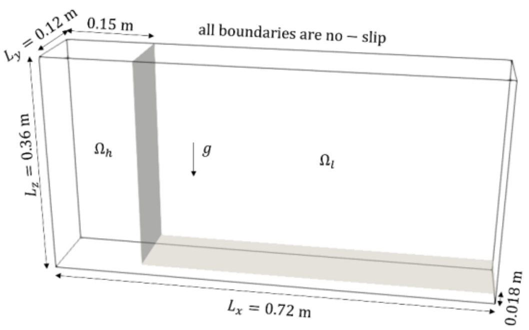

Fig. 4 Schematic of the initial condition of 3D dam-breaking problem on a wet floor.

Fig. 4 shows the problem setup. An initial stationary water column with a width of 15 cm and height of 36 cm is placed touching the ceiling at the left-end of the domain. The height of the thin water layer is 1.8 cm which corresponds to a depth ratio of 0.05. The physical parameters of this problem are the same as in the previous dam-breaking problem. The reference velocity and Reynolds number are defined as:

$$u_0 = \sqrt{gh} \approx 1.83 \ \frac{\mathrm{m}}{\mathrm{s}}, \tag{28}$$

$$Re = \frac{\rho_h u_0 h}{\mu_h} \approx 6.3 \times 10^5. \tag{29}$$

The problem was simulated up to time $T = 1$ s with a resolution of $N_x \times N_y \times N_z = 576 \times 288 \times 96$ and a time interval $\Delta t = 1/80000$. The reference employs a high resolution of $1024 \times 512 \times 176$.

Fig. 5 shows the evolution of the water profile obtained by the filtered CLBM (right) and the reference (left). As soon as the flow is released, a wave is developed at 0.2 s, interacts with the down-stream water (wave-breaking) at 0.3 s, entrains air at 0.4 s, and then crashes against the right-end of domain at 0.5 s. The results from the proposed method are qualitatively in good agreements with the reference although they look more viscous due to the application of diffuse interface model and second order filter.

Fig. 6 shows the present result at later stages which show that the proposed method remains stable at later stages. These results are unavailable in the reference [19]. During these later stages, the entrained air develops into many bubbles which rise up to the surface. The water splashing on the ceiling develops into many droplets which fall, break, and recombine. After it rises, the wave then returns with many small droplets raining on it, which could make the simulation using other two-phase LBMs unstable.

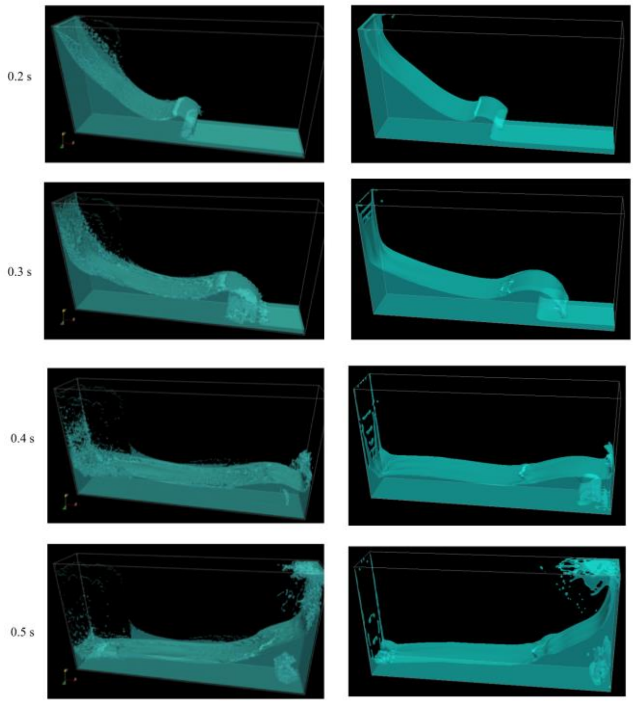

Fig. 5 Evolution of water profiles in 3D dam-breaking on a wet floor. Reference (left) and filtered CLBM (right).

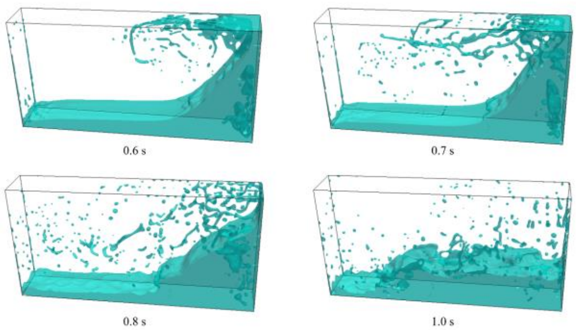

Fig. 6 Evolution of water profiles in 3D dam-breaking on a thin film at later stages.

3.2. 3D oblique coalescence of two-bubbles

The 3D oblique coalescence of two bubbles problem is considered. The schematic of the problem is shown in Fig. 7. Two spherical bubbles, identical in size with diameter $d = 0.01$ m, are arranged in oblique configuration as shown in the figure. The density and viscosity of the heavy phase are $\rho_h = 100\ \mathrm{kg/m^3}$ and $\mu_h = 4.63 \times 10^{-3}\ \mathrm{kg/(m \cdot s)}$, whereas the density and viscosity of the light phase are $\rho_l = 1\ \mathrm{kg/m^3}$ and $\mu_l = 4.63 \times 10^{-5}\ \mathrm{kg/(m \cdot s)}$. The Morton and Eotvos numbers for this case are defined as:

$$M = \frac{g {\mu_h}^4 \Delta\rho}{\rho_h^2 \sigma^3} = 2 \times 10^{-4}, \tag{30}$$

$$Eo = \frac{\Delta\rho g d^2}{\sigma} = 16, \quad (31)$$

where g is the gravity, σ is the surface tension, and $\Delta\rho = \rho_h - \rho_l$.

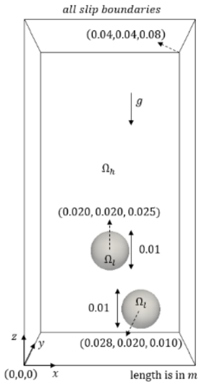

Fig. 7. Schematic of initial condition of the 3D oblique coalescence of two bubbles.

The problem is solved using both unfiltered and filtered CLBM on a mesh of $N_x \times N_y \times N_z = 80 \times 80 \times 160$ gridpoints, where N_x, N_y, N_z are the number of mesh in x-, y-, z-direction, respectively, and $N_t = 4000$ time steps.

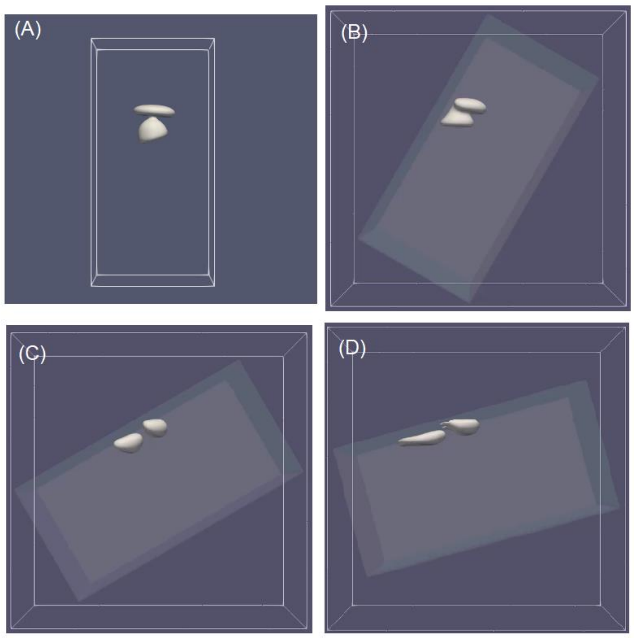

Fig. 7 Bubble shapes at *t*=1.5 s in 3D oblique coalescence of two bubbles in inclined channel. (A) 90º (B) 60º (C) 45º (D) 30º.

Fig. 7 shows a snapshot of bubble shapes at *t*=1.5 s for various inclinations. In our preliminary study, the proposed method capable to stably solve this problem and conserve the mass within the machine error. The bubble shape obtained in Fig. 7 (A) is in a good agreement with the experimental data by Brereton and Korotney [20]. By changing the inclination, different bubble shapes are obtained where the bubbles are not only interact to each other but also interact with the wall boundaries.

4. Conclusions

This work presents a novel filtered cumulant lattice Boltzmann method (filtered CLBM) which has been developed to solve violent two-phase flow problems, such as the dam-breaking setting. The proposed method employs the velocity-based formulation of the two-phase LBM which has better stability than the momentum-based formulation, as the pressure update has less incompressibility error and the velocity update is done semi-implicitly. The cumulant collision model is also employed which has a good stability for problems with high Reynolds number. To further enhance the stability for the simulation of violent two-phase flows, a second order hybrid-like filter is also employed and can be turned off for non-violent flows. This filter adds artificial viscosity which depends on the flow Peclet number similarly to the hybrid differencing scheme for the advection equation. The algorithm is completed by the conservative phase-field lattice Boltzmann method (CLBM) which used for interface capturing and guarantees mass conservation.

The proposed method, along with its unfiltered version, has been validated on two non-violent two-phase flow problems, namely the 2D rising bubble and the 3D droplet splashing on a thin film. The results show good agree-ments with both computational and experimental references. The proposed method has however a low order ac-curacy due to the application of filter and therefore high resolution is needed for sufficient accuracy, as seen in the 3D droplet splashing on a thin film problem. The proposed method has been applied to simulate the dam-breaking which show its capacity in handling violent two-phase flows. The results show qualitative agree-ments between the proposed method and the computational references. A preliminary study is also conducted to simulate two-phase flow problem in complex geometry. An oblique coalescence of two bubbles in inclined channel is considered. In this simulation the mass is conserved up to the machine error. The proposed method is capable to stably solve this problem. Future study may include the simulation of turbulent bubbly flows in inclined channel.

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