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Three-dimensional lattice Boltzmann simulation of bubble behavior in a flap-induced shear flow

Zhikai Wang [a,*], Dongyan Shi [a], Aman Zhang [b]

[a] College of Mechanical and Electrical Engineering, Harbin Engineering University, Harbin 150001, China
[b] College of Shipbuilding Engineering, Harbin Engineering University, Harbin 150001, China

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ABSTRACT

Based on the kinetic nature of the lattice Boltzmann method (LBM), the critical part of simulating a bubble in a shear flow is focused on two types of boundaries, i.e., the fluid-structure boundary and the gas–liquid interface. Based on the free-energy model, two particle distribution functions are defined for the fluid density and an order parameter, separately. The gas–liquid interface can be described by solving the Cahn–Hilliard equation, then a modified bounce-back boundary treatment is used for the fluid-structure boundary. During the bounce-back process, the effect of boundary moving velocity is taken into account in calculating the two distribution functions. By the above processing, a three-dimensional numerical model is established to predict bubble behaviors in a flap-induced shear flow, which takes the effect of the presence of solid boundaries into consideration. Due to the coexistence of three phases, a detailed verification including the multiphase Laplace Law, the mass conservation, the bubble deformation and the shear flow property is completed in the wall-bounded shear flow. Subsequently, the effects of flap velocity and fluid viscosity which are both related to the capillary number are investigated. The fact that the capillary number could not able to predict the bubble deformation well theoretically due to the existence of solid boundaries is confirmed. These results show that the flap velocity and the fluid viscosity affect the transient deformation process more severely than flow patterns.

1. Introduction

The flow-induced deformation research of a bubble is an important component in fluid dynamics, not only due to its wide existence in the industrial field but because of its essential position in the fundamental research. Traditionally, the flow structure around a bubble is not stable, and has a complex velocity property. A typical and simplified situation is that a bubble moves and deforms in a shear flow. Then, further research works can be promoted to model more complex situations.

Two important issues in simulating a bubble in a shear flow are the bubble interface treatment and the fluid-structure boundary treatment. In the related areas, the subject of elastic membrane movement has been studied extensively for a long time. Starting from the pioneering work by Taylor [42], most literatures on flow-induced drop or bubble simulations are devoted to the unbounded flows, where the wall effect can be ignored. Schmid-Schoenbein and Well [30] carried out the work by experimental studies. Barthes-Biesel et al. [4, 5] tried to explain the deformation of an elastic deformation by theoretical analysis. Shapira et al. [32] theoretically analyzed the hydrodynamic interaction between the bubble in shear flows and the two boundary walls. However, it is well known that though some features are similar, the gas–liquid interface is different from an elastic capsule for its constant surface tension. Sheth and Pozrikidis [33] conducted numerical simulations to study the effects of inertia on the deformation of liquid drops in simple shear flows. Subsequently, Lee and Pozrikidis [19] researched the bubble interface deformation in Navier–Stokes flows. Zhang and Li [49,50] carried out some studies on bubble oscillation and mass diffusion under the condition of acoustic excitation. With the development of high performance computing and various numerical methods, numerical simulations are playing a more important role in the field of bubble dynamic research. In the conventional numerical methods, the volume-of-fluid (VOF) method is one of the most popular methods. Rabha and Buwa [26] simulated single/multiple bubbles in sheared liquids by using the VOF. Another popular method is the boundary element method (BEM) which can effectively conserving computing resources. Based on the BEM, Zhang et al. carried out further studies on bubble motions under various conditions, such as the fluid viscosity, the compressibility and the different solid boundary conditions [21, 46–48].

* Corresponding author. Tel.: +86 045182518296; fax: +86 45182518296.
E-mail address: zhikai.wa@gmail.com, zhangaman@hrbeu.edu.cn (Z. Wang).

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For moving fluid-structure boundary treatments, some matters should be paid more attention. It is the origination of the flap-induced shear flow [38]. Through the experimental study, Sibillo et al. [35] investigated the bubble deformation under the condition of both considering and ignoring wall effects. The most important issue in Sibillo's work is that a clear picture of drop deformation in the confined shear flow is given. Meanwhile, Sibillo's work indicates that the Taylor theory (1934) is not suitable for the bubble deformation prediction in a wall-bounded shear flow. In addition, the effect of the non-dimensional gap ratio ranging from 0.07 to 1 was researched. It was found that the higher the gap ratio, the more extended is the shape at steady state. Driven by Sibillo's work, a three-dimensional model of simulating a bubble in wall-bounded shear flows is established based on the Lattice Boltzmann method. The density and momenta is conserved by describing a set of particles moving on a Euler grid at each step thus approximating the behavior of the hydrodynamic equations for the fluids [45]. It has been reported that the LBM has a comparative advantage in dealing with complex boundaries including multiphase interfaces [3,7,25] and fluid-structure boundaries [17,53] based on its molecular kinetic theory characteristics. The most famous four models for immiscible two-phase flows are: Shan-Chen model [31], Rothman-Keller model [9], mean-field model [12,13], and Free energy model [14,40].

In present study, the whole model is based on the free-energy lattice Boltzmann BGK model such that bubble interface deformations and fluid properties are determined by the free energy. By solving the convective Cahn–Hilliard equation instead of the scalar transport equation, the interface profile can be analytically introduced into the free energy function, which can overcome the deficiencies of the work of Inamuro et al. [14] and Swift et al. [40]. In addition, special treatments of fluid-structure boundaries are completed to introduce the effects of boundary motions and offsets on the accuracy of the calculated results when actual physical borders and grid lines do not coincide in the multiphase flow system.

2. Computational model and implementation

For wall-bounded shear flows, Lee et al. [19] proposed a two-dimensional model to simulate the bubble motion. Based on the dual grid lattice Boltzmann method, Rosales et al. [27] studied the effect of the gap ratio (R/H, R is the bubble radius, and H is the channel height) on bubble deformations in a wall-bounded shear flow. Rosales found that when the ratio was 0.1, the effect of the channel walls was expected to be minimal, and the numerical results matched well with the theoretical predictions by Cox [6]. When the ratio increased to 0.2, 0.333, the results would have a significant deviation, though *Ca* was still kept as 0.05. However, Rosale's work was based on the two-dimensional model, so the consequence of dropping the third dimension was not completely known, and a clear picture of drop deformation in confined shear flow was still lacking. In our work, a three-dimensional model is established. Meanwhile, a clear view of bubble deformations and fluid profiles is given.

2.1. Three-dimensional computational model

A bubble is immersed in the shear flow induced by the top and bottom moving flaps with the velocity, $u_{1x} = u_b$, $u_{1y} = 0$. The simulated system consists of one bubble with a certain interface thickness situated in the center of a $H \times L \times W$ domain, as shown in Fig. 1. The bubble interface is N, and the surface tension coefficient is defined as σ. The lattice unit system in the work of Zheng et al. [52] is referred in present study. Therefore, the uniform mesh is used with $\Delta x = \Delta y = \Delta z = 1$, and the time interval Δt equals to the spatial mesh spacing. That said, the lattice unit is always kept as 1 and the lattice time is actually the time steps.

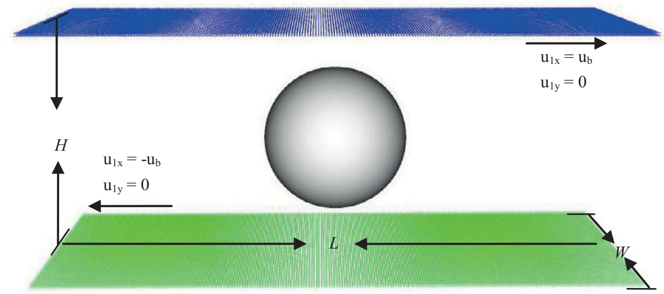

Fig. 1. Model sketch of bubble initialized in the gap of two moving flaps.

For the two phases, their movements can be described by the Navier-Stokes equations:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$
$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = -\nabla \cdot \mathbf{P} + \mu \nabla^2 \mathbf{u} + \mathbf{F}. \quad (1)$$

The interface evolution can be obtained by solving the Cahn–Hilliard equation ([15]; Kendon et al. [16]):

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\phi \mathbf{u}) = M \nabla^2 \theta. \quad (2)$$

Here, ϕ is the order parameter [41] defined as $|\rho_1 - \rho_2|/2$. M is the mobility and θ is the chemical potential that can be calculated according to the free-energy model.

2.2. Bubble interface representation

To solve the Cahn–Hilliard equation, a modified lattice Boltzmann equation [18] is adopted by following the work of Zheng et al. [51,52]:

$$f_i(\mathbf{x} + \mathbf{e}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + (1 - q)[f_i(\mathbf{x} + \mathbf{e}_i \Delta t, t) - f_i(\mathbf{x}, t)] + \Omega_i. \quad (3)$$

where f_i is the particle distribution function, $\mathbf{e}_i$ is the lattice discrete velocity, and q is the constant coefficient. Ω_i is the collision term which can be written as

$$\Omega_i = \frac{f_i^{eq}(x, t) - f_i(x, t)}{\tau_\phi}. \quad (4)$$

where τ_ϕ is the dimensionless relaxation time parameter, f_i^{eq} is the equilibrium distribution function. By using Taylor series expansion, Eq. (3) can be written as

$$\Delta t(\partial_t + \mathbf{e}_i \cdot \nabla) f_i + \frac{1}{2}(\Delta t(\partial_t + e_i \cdot \nabla))^2 f_i$$
$$= (q - 1)(\Delta t(e_i \cdot \nabla) f_i + \frac{1}{2}(\Delta t(e_i \cdot \nabla)^2 f_i) + O((\Delta t)^3) + \Omega_i \quad (5)$$

Furthermore, by using the Chapman-Enskog expansion,

$$f_i \approx f_i^{eq} + \varepsilon f_i^{(1)} + \varepsilon^2 f_i^{(2)}$$
$$\partial_t \approx \varepsilon \partial_{t0} + \varepsilon^2 \partial_{t1}, \quad (6)$$
$$\partial_x \approx \varepsilon \partial_{t1}$$

where ε is the Knudsen number, the Cahn–Hilliard equation with the second order of accuracy can be recovered,

$$\partial_t \phi + \nabla \cdot (\phi \mathbf{u}) - M \nabla^2 \theta + O((\Delta t)^2) = 0, \quad (7)$$

where $M = (2\tau_\phi q^2 - q)\Gamma \Delta t/2$ and $q = 2/(2\tau_\phi + 1)$. Γ is a parameter used to modify the mobility. In the calculation process, the following