Chemical Engineering Science 65 (2010) 5615–5623

Contents lists available at ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

A modified pseudopotential for a lattice Boltzmann simulation of bubbly flow

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ARTICLE INFO

Article history:
Received 6 August 2009
Received in revised form
2 July 2010
Accepted 10 August 2010
Available online 13 August 2010

Keywords:
Lattice Boltzmann model
Pseudopotential
Bubbly flow
Gas–liquid density ratio
Spurious velocity
Equation of state

ABSTRACT

The pseudopotential in Shan and Chen-type multiphase models was investigated and modified based on a virial equation of state with newly proposed parameters. This modified pseudopotential was used in a lattice Boltzmann model and shown to be suitable for simulating sufficiently large gas–liquid density ratios with good numerical stability and only small spurious velocities. The spurious velocity was reduced by reducing the pseudo-sound speed by the use of suitable parameters. The multicomponent multiphase model based on this modified pseudopotential can be used in bubbly flow simulations. Bubble rise behavior was simulated using a 3D multicomponent and multiphase model with a high density ratio. The predicted terminal velocity and drag coefficient of a single bubble agreed well with those calculated from empirical correlations. The drag coefficient of bubbles in the homogenous regime decreased with increased gas holdup. A new relationship between the bubble drag coefficient and gas holdup in the homogenous regime was proposed.

1. Introduction

In recent years, the lattice Boltzmann method (LBM) has become an alternative and attractive approach to simulate fluid flow and transport phenomena, especially in complex and multiphase media. It is considered an effective simulation method on the mesoscale because the microscopic forces can be directly included in its description of interfacial phenomena of the bubbles and droplets. Házi et al. (2002), in a review of lattice Boltzmann models for gas–liquid simulations, divided them into three types: color models (Gunstensen et al., 1991), pseudopotential models (Shan and Chen, 1993; He et al., 1999) and free energy models (Swift et al., 1996). These models distinguish two different kinds of matter or state on the basis of a parameter. Among these models, the pseudopotential model is the most widely used due to its simplicity and high computational efficiency (Sukop and Thorne, 2006).

However, most LBM models for bubble simulation are still limited to conditions of low bubble Re, Mo, or Eo numbers due to the limitation to a low density ratio, and the problems of large spurious velocities and poor numerical stability. Many previous works have suggested ways to improve the LBM for use with higher gas–liquid density ratios for bubble simulations. Inamuro et al. (2004) proposed a method for simulating two-phase flows with a large density ratio of 1000 by solving the pressure Poisson equation with free energy. However, it was very time consuming to solve the pressure Poisson equation. Lee and Lin (2005) used the pressure evolution equation and simulated two-phase flows with a density ratio of 1000. In their model (Lee and Lin, 2005), the discretization of the collision step was different before and after the streaming step, which also carried additional computational costs. Zheng et al. (2006) reported that high liquid–gas density ratios can be realized by using an interface-capturing scheme based on the Cahn–Hilliard equation. However, the density ratio in their model (Zheng et al., 2006) was for the two components, and not for the two phases. The two phases had the same density in their model (Zheng et al., 2006). Most recently, Lishchuk et al. (2008) reported a method for simulating gas–liquid flow with high density ratios by introducing effective shear-dependent forces acting in the region of the interface. All the above methods introduced an additional treatment to the original Shan and Chen-type model (Shan and Chen, 1993; He et al., 1999), such as a pressure Poisson equation, different discretization steps, interface capturing process and shear dependent forces. These treatments increase the complexity and computational cost of the simulation, which were at odds with the concise nature of the LBM.

There have also been many previous works for reducing the spurious velocity. Nourgaliev et al. (2002) found that the spurious velocity could be reduced with a finite difference approach in the streaming step. Wagner (2003) argued that that the spurious velocity was caused by non-compatible discretization of the driving forces, and reduced the maximum spurious velocity to $O(10^{-16})$ using the potential form of the surface tension. However, a numerical viscosity correction term had to be added

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doi:10.1016/j.ces.2010.08.014

due to numerical instability. Lishchuk et al. (2003) reported that the spurious velocity was due to the microscopic nature of the LBM in which the interface had a finite thickness. They incorporated a sharp interface into the kinematics to reduce the spurious velocity. Cristea and Sofonea (2003) found that the directional derivative operator was the main reason for the spurious velocity in the interfacial region. Lee and Fischer (2006) reported that the spurious velocity could be eliminated by using the potential form of the intermolecular force with a compact isotropic discretization. Shan (2006) showed that the spurious velocity was caused by insufficient isotropy of the discrete gradient operators and could be reduced by using highly isotropic gradient operators. All these previous works had to include some additional treatments, e.g., a finite difference streaming step, numerical viscosity correction, sharp interface kinematics or highly isotropic gradient operators to reduce the spurious velocity.

The interaction potential, which determines the equation of state of the fluid, has important effects on the density ratio range and spurious velocity of pseudopotential-based single component multiphase LBMs. Yuan and Schaefer (2006) performed static simulations with a density ratio of 1000 by using an appropriate interaction potential. They did not need to use complicated discretization or solve the Poisson equation, but only static cases without gravity were investigated. In fact, when the vapor density was too low, the dynamic simulation was not easy. Yu and Fan (2007) also proposed a new expression for the potential between species that allowed the use of the multicomponent multiphase model with high density ratios that reached steady state quickly. These works showed that an improvement of the interaction potential expression based on a modification of the equation of state would be helpful for improving the pseudopotential model in bubbly flow simulation and to simulate bubble dynamics with gravity. The objectives of the current study were to study the influence of the equation of state on the LBMs for bubble simulation, and to propose a new equation of state that can be used for sufficiently large gas–liquid density ratios, which also gave a small spurious velocity and good numerical stability. The paper is organized as follows. A brief description of the theoretical basis of the LBM with a pseudopotential model is given first. Then different pseudopotential models are compared and an improved pseudopotential model is proposed with an equation of state with new parameters. Simulation results of bubbly flow are given and verified by experimental results. Finally, a new relationship between the bubble drag coefficient and gas holdup in the homogenous region is proposed based on the simulation results.

2. Methodology

2.1. The pseudopotential LBM

In a standard LBM without a force, the evolution of the particle distribution is described by the equation

$$f_i(\mathbf{x}+\mathbf{e}_i\Delta t,t+\Delta t)-f_i(\mathbf{x},t)=-\frac{1}{\tau}\left[f_i(\mathbf{x},t)-f_i^{eq}(\mathbf{x},t)\right] \quad (1)$$

In the simplest implementation, with $\delta x=\delta t=1$, the equilibrium distribution function is expressed as

$$f_i^{eq}(\rho(\mathbf{x}),\mathbf{u}^{eq})=w_i\rho(\mathbf{x})\left[1+3\mathbf{e}_i\cdot\mathbf{u}^{eq}+4.5(\mathbf{e}_i\cdot\mathbf{u}^{eq})^2-1.5(\mathbf{u}^{eq})^2\right] \quad (2)$$

where w_i is the weight factor, and $\mathbf{u}^{eq}$ is the equilibrium velocity. The equilibrium velocity is affected by the interacting force $\mathbf{F}$ that is manifested in a nonideal equation of state of the fluid and external forces. In this work, only the gravity force was considered in the external forces. Thus, the equilibrium velocity can be expressed as (Guo et al., 2002)

$$\mathbf{u}^{eq}=\frac{1}{\rho}\left[\sum_i f_i\mathbf{e}_i+\tau\mathbf{F}(\mathbf{x})\right] \quad (3)$$

$$\mathbf{F}(\mathbf{x})=\mathbf{F}_{gravity}(\mathbf{x})+\mathbf{F}_{int}(\mathbf{x}) \quad (4)$$

The gravity force was formulated as (Sankaranarayanan et al., 2002)

$$\mathbf{F}_{gravity}(\mathbf{x})=\mathbf{g}\cdot[\overline{\rho}-\rho(\mathbf{x})] \quad (5)$$

The density and velocity were calculated as

$$\rho=\sum_i f_i \quad (6-a)$$

$$\rho\mathbf{u}=\sum_i f_i\mathbf{e}_i+\tfrac{1}{2}\mathbf{F}(\mathbf{x}) \quad (6-b)$$

The fluid momentum is defined as the average of the momentums before and after collision (Shan and Chen, 1994). There are also other approaches for incorporating the interaction force, such as direct body forcing. The interaction force $\mathbf{F}_{int}(\mathbf{x})$ was associated with the nonideal equation of state of the fluid, and was obtained by the pseudopotential model. $\mathbf{F}_{int}(\mathbf{x})$ was an interaction force between nodes, which was the driving force for phase separation. The macroscopic Navier–Stokes equations can be derived by Chapman–Enskog expansion from Eqs. (1)–(6) with approximation to the second order (Guo et al., 2002):

$$\frac{\partial\rho}{\partial t}+\nabla\rho\mathbf{u}=0 \quad (7-a)$$

$$\frac{\partial}{\partial t}(\rho\mathbf{u})+\nabla\cdot(\rho\mathbf{u}\mathbf{u})=-\nabla\mathbf{P}+v\nabla\left[\rho(\nabla\mathbf{u}+(\nabla\mathbf{u})^T\right]+\mathbf{F} \quad (7-b)$$

where the viscosity $v=1/3(\tau-0.5)$ in the D2Q9 model. The hydrodynamic pressure $\mathbf{P}$ in Eq. (7-b) satisfies the thermodynamic equation of state from the detailed deducing process, so hydrodynamic pressure is equivalent to the thermodynamic pressure in the bulk of each phase (He and Doolen, 2002; Shan, 2008).

2.2. Interaction potential in pseudopotential model

The pseudopotential-based LBM was first proposed by Shan and Chen (1993, 1994). In physical chemistry, the intermolecular potential is often approximated by the Lennard–Jones potential, but this cannot be directly used in LBM because each LB particle contains a large number of molecules. Shan and Chen (1993, 1994) used the nearest neighbor interaction potential to approximate the intermolecular potential. The interaction potential was modeled as

$$V(\mathbf{x},\mathbf{x}+\mathbf{e}_i)=Gw_i\psi(\mathbf{x})\psi(\mathbf{x}+\mathbf{e}_i) \quad (8)$$

and the interparticle force could then be calculated as

$$\mathbf{F}_{int}(\mathbf{x})=-G\psi(\mathbf{x})\sum_{i=1}^{n}w_i\psi(\mathbf{x}+\mathbf{e}_i)\mathbf{e}_i \quad (9)$$

where G is the strength of the interparticle potential, n is the number of involved neighbors, ψ is a function of particle density and w_i is the weight factors.

Using the mean field approximation for intermolecular attraction and the method of treating the exclusion volume effect proposed by Enskog, He et al. (1999) obtained the expression for