International Communications in Heat and Mass Transfer 87 (2017) 183–191

Contents lists available at ScienceDirect

International Communications in Heat and Mass Transfer

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

Study on multicomponent pseudo-potential model with large density ratio and heat transfer

Weibing Zhu, Meng Wang*, Hong Chen

College of Aerospace and Civil Engineering, Harbin Engineering University, Harbin 150001, China

ARTICLE INFO

Keywords:
Pseudo-potential model
Large density ratio
Spurious current
Thermal multiphase flow

ABSTRACT

Large density ratio multiphase flow is a persistent challenge within the field of computational fluid dynamics. This paper investigates improvements to the lattice Boltzmann based large density ratio multicomponent multiphase pseudo-potential model. The improvements include: the multiple-relaxation-time (MRT) collision operator; the exact difference method scheme; the Carnahan-Starling equation of state; and an addition of correction factor k to the equation of state. The improved model can be used for simulating large density ratio (O(1000)) multiphase flow with small spurious current and better numerical stability. The smaller spurious current can be obtained by decreasing k value, and yet interface thickness increases. The density ratio is 1284 for $k = 0.1$ and the spurious current is reduced to 0.0069, which is much smaller than that of 0.033 in literature. The interfacial tension can be adjusted independently from density ratio by changing k value. A thermal multiphase flow model is developed based on the large density ratio pseudo-potential model. The model is validated by using static heat conduction and dynamic flow simulations. The result of the static heat conduction of the flat interface has smaller error with the theoretical solution than that of droplet. The result of thermocapillary migration is comparable with the theoretical prediction. Finally, the heat conduction melting is simulated by coupling the enthalpy-based method.

1. Introduction

Multicomponent multiphase flow exists extensively in a range of application fields such as: the oil-gas separation process in the aero-engine oil system [1]; the extraction and transportation process of natural gas and petroleum [2]; the evaporation in the boiler [3] and the condensation in the condensator. In the ablation process of C/SiC composites applied to solid rocket engine nozzle, SiC is oxidized to SiO_2 and then melted under the working temperature of rocket engine [4]. Multicomponent gas and the liquid SiO_2 constitute multiphase flow system, which is a complicated physiochemical process involving heat transfer, phase change, multiphase flow, and chemical reaction. In traditional computational fluid dynamics (CFD), the level-set method and the volume of fluid (VOF) method have been successfully used for the simulation of multiphase flow [5]. However, these require complex interface tracking or capture technology, and interactions cannot be considered among the constituent molecules in microscopic scale.

The lattice Boltzmann method (LBM), a mesoscopic method, developed over the past two decades, is derived from the lattice gas automata (LGA) method. The LBM has some attractive advantages, such as its simple model, convenience for handling complex geometry and boundary, and the inherent parallel nature. It has been used to address various complex fluid flow problems, including porous media flow, multicomponent and multiphase flow, chemical reaction, and micro-scale gas flows [6]. Multiphase models in the LBM belong to diffuse interface method, in which the sharp phase interface is replaced by a narrow layer of fluid mixtures [7]. In several models, the pseudo-potential model (also known as the Shan-Chen model) [8–10], proposed by Shan and Chen, is the most widely used model due to its simplicity [11,12]. A mean field force replaces the intermolecular interactions in the pseudo-potential model, thus the gas phase and liquid phase can be separated. However, there are some deficiencies with the original pseudo-potential model. One of deficiencies is that it is incapable for the simulation of large density ratio (it can only achieve a maximum density ratio of the order of O(10)). However, large density ratio exists in the vast real-world multiphase flow systems, such as the oil-gas separation and the ablation process previously described, in which the density ratio exceeds 1000. Yuan and Schaefer [13] introduced several equation of state (EOS) of non-ideal gas to pseudo-potential model, and the density ratio can be raised to 1000. Kupershtokh et al. [14] integrated reduced equations of state into pseudo-potential model, and combined effective mass method and Zhang and Chen's method [15] for

* Corresponding author.
E-mail addresses: wangmengnmg@hrbeu.edu.cn, wangmengnmg@gmail.com (M. Wang).

http://dx.doi.org/10.1016/j.icheatmasstransfer.2017.07.007

the calculation of the interaction force. The larger density ratio can be achieved. Subsequently, Kupershtokh [16] introduced a dimensionless coefficient k into the reduced equation of state to improve numerical stability. Hu et al. [17] modified vdW equation of state by incorporating a similar coefficient k. Hu et al. indicated that the smaller spurious current and better numerical stability can be achieved by reducing the value of k, and the surface tension can be adjusted by changing the value of k. Recently, Stiles and Xue [18] took the same approach (they called it k method) to the Peng–Robinson EOS. They focused on the effect of coefficient k on interface thickness, temperature ranges, spurious velocities and stability. They pointed out that the lowest temperature results should be discarded due to the non-physical density variations along the phase interface. Liu et al. [19] incorporated the virial equation of state and modified parameters, which could decrease the spurious current by reducing the pseudo-sound speed.

Above-mentioned studies are improvements about single component pseudo-potential model. Bao and Schaefer [20] incorporated the equation of state of non-ideal gas into multicomponent pseudo-potential model, and the density ratio can also be enhanced to 1000. Furthermore, a few studies also focused on increasing the density ratio for multicomponent systems [18,19,21–23]. We can find out that adopting the real equation of state is an effective means to improve density ratio. The spurious current in the vicinity of phase interface is also one of drawbacks of the original pseudo-potential model. This is because the restricted discretization in calculating interaction force brings about imbalance between the pressure difference and the surface tension [11]. Therefore, the spurious current cannot be eliminated, and it can only be reduced to an acceptable range. The spurious current increases as density ratio increases, which is a significant cause of disability of the original pseudo-potential model for large density ratio. Except for employing the real equation of state, following methods can be used for decreasing the spurious current: (1) adopting the multiple relaxation time (MRT) collision operator. The spurious current can be effectively reduced by adjusting free parameters of MRT [24,25]. (2) Adopting the interaction force with high order isotropy. Only the nearest neighbor nodes are used for calculating interaction force in the original pseudo-potential model. The interaction force with high order isotropy involves more discrete directions, consequently the spurious current is weakened [25–27]. (3) Adopting the suitable force schemes. The spurious current [28,29] can be reduced by using Guo's force scheme [30] and the exact difference method (EDM) scheme [31]. (4) Using refined grid [27] and wider interface thickness [32] can also decrease the spurious current.

The above studies are specific to the isothermal system, but heat transfer is often involved in the real-world multiphase flow systems. To the best of our knowledge, few studies have focused on thermal multicomponent multiphase flow in literatures. Parmigiani et al. [33] combined the multicomponent pseudo-potential model with the enthalpy-based method to simulate the multiphase flow with melting problems. The effects of Stefan number on the non-wetting fluid invading porous media were investigated. Qiu et al. [34] studied natural convection of two immiscible fluids in a square cavity, and analyzed the influence of Rayleigh number. The density ratio is equal to 1 in Parmigiani et al. and Qiu et al.'s works, and single temperature equation was used for describing heat transfer of multicomponent. Ikeda et al. [35] proposed a thermal multicomponent model based on the large density ratio pseudo-potential model. In their model, the each component employs respective temperature equation, and then the temperature is coupled at each node using density-weighted combination.

Although scholars have enhanced the density ratio of multicomponent pseudo-potential model, the drawbacks of the large spurious current and numerical instability still exist. In order to reduce the spurious current and increase the stability of the model, based on the previous studies in literatures, we improve multicomponent pseudo-potential model with large density ratio by the following methods: the MRT model is used for approximating the collision operator; the exact difference method is adopted for the external force scheme; the Carnahan-Starling equation of state is incorporated into pseudo-potential model; and a correction factor k is added to the equation of state for adjusting the parameters. Further, we develop the thermal multicomponent multiphase flow model with large density ratio based on the single temperature equation. Finally, we make research on the conduction melting problem by combining the enthalpy-based method.

2. Simulation of multicomponent multiphase flow with large density ratio

2.1. Pseudo-potential lattice Boltzmann model

The MRT model [36] is adopted for the collision operator. Collision process is carried out in the moment space, while streaming process is performed in the velocity space. The evolution equation of the density distribution function is expressed by

$$\mathbf{f}_\sigma(\mathbf{x}+\mathbf{e}_i\delta_t, t+\delta_t) - \mathbf{f}_\sigma(\mathbf{x},t) = -\mathbf{M}^{-1}\mathbf{S}_\sigma[\mathbf{m}_\sigma(\mathbf{x},t) - \mathbf{m}_\sigma^{eq}(\mathbf{x},t)] + \mathbf{F}_\sigma(\mathbf{x},t) \tag{1}$$

where $\boldsymbol{f}_\sigma(\boldsymbol{x},t)$ is the vector form of density distribution function of σ component at the site $\boldsymbol{x}$ and time t. For D2Q9 model, $\boldsymbol{f}_\sigma = (f_0, f_1, \cdots, f_N)^{\mathrm{T}}$ ($N = 8$). δ_t is the time step. $\boldsymbol{e}_i$ is the discrete velocities, and it can be determined by

$$\mathbf{e}_i = c\begin{bmatrix} 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \end{bmatrix} \tag{2}$$

where $c = \delta_x/\delta_t$ is the lattice velocity, and δ_x is the lattice spacing. $\boldsymbol{M}$ is the transform matrix [37]. $\boldsymbol{m}$ and $\boldsymbol{m}^{eq}$ are the distribution function and the equilibrium distribution function in the moment space, respectively.

$$\mathbf{m} = (\rho, e, \varepsilon, j_x, q_x, j_y, q_y, p_{xx}, p_{xy})^{\mathrm{T}} \tag{3}$$

$$\mathbf{m}^{eq} = (\rho, -2\rho + 3(u_x^2 + u_y^2), \rho - 3(u_x^2 + u_y^2), u_x, -u_x, u_y, -u_y, u_x^2 - u_y^2, u_x u_y)^{\mathrm{T}} \tag{4}$$

The macroscopic density ρ_σ and velocity $\boldsymbol{u}_\sigma$ of σ component are calculated as

$$\rho_\sigma = \sum_i f_{\sigma,i} \qquad \rho_\sigma \mathbf{u}_\sigma = \sum_i f_{\sigma,i}\mathbf{e}_i \tag{5}$$

$\boldsymbol{S}$ is the relaxation matrix, and it can be written as

$$\mathbf{S} = \mathrm{diag}(1, s_e, s_\varepsilon, 1, s_q, 1, s_q, s_v, s_v) \tag{6}$$

If all values of s_i are identical, the MRT model will reduce to the Lattice Bhatnagar–Gross–Krook (LBGK) model. We set $s_e = s_\varepsilon = s_v$, $s_q = 8(2\text{-}s_v)/(8\text{-}s_v)$ [38]. s_v is used for determining the shear viscosity.

$$\nu = c_s^2\left(\frac{1}{s_\nu} - \frac{1}{2}\right)\delta_t \tag{7}$$

where $c_s = 1/\sqrt{3}$ is the lattice sound velocity. $\boldsymbol{F}_\sigma = (F_{\sigma 0}, F_{\sigma 1}, \cdots, F_{\sigma N})^{\mathrm{T}}$ is the external force term for the component σ. We adopt the exact difference method (EDM) scheme proposed by Kupershtokh [31] to implement the external force into the LB framework. The EDM scheme is derived directly from the Boltzmann equation, and the force term in the evolution equation is given by

$$F_{\sigma,i} = f_{\sigma,i}^{eq}(\rho_\sigma, \mathbf{u}^{eq} + \Delta\mathbf{u}_\sigma) - f_{\sigma,i}^{eq}(\rho_\sigma, \mathbf{u}^{eq}) \tag{8}$$

where f^{eq} is the equilibrium distribution function, $\boldsymbol{u}^{eq}$ is the equilibrium velocity. $\Delta\boldsymbol{u}_\sigma = \boldsymbol{F}_{\sigma,total}\delta t/\rho_\sigma$, $\boldsymbol{F}_{\sigma,total}$ is the total force acting on σ component. $\boldsymbol{u}^{eq}$ is calculated by

$$\mathbf{u}^{eq} = \sum_\sigma \rho_\sigma \mathbf{u}_\sigma \Big/ \sum_\sigma \rho_\sigma \tag{9}$$

Because the MRT model is employed, for convenience, we rewrite Eq. (8) as follows