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An optimal two-relaxation-time lattice Boltzmann equation for solid-liquid phase change: The elimination of unphysical numerical diffusion

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ABSTRACT

This paper proposes an optimal two-relaxation-time (OTRT) lattice Boltzmann equation (LBE) for solid-liquid phase change. By using the Chapman-Enskog expansion, the OTRT LBE can recover the enthalpy-based energy governing equation up to second-order accuracy. Moreover, a detailed theoretical analysis proves that by keeping an optimal relation between the two relaxation times, the OTRT LBE can effectively eliminate the unphysical numerical diffusion of arbitrary D*m*Q*n* (*m* dimensions and *n* discrete velocities) lattice Boltzmann models for both one-phase and two-phase melting problems. Five test cases including one-dimensional to three-dimensional solid-liquid phase change problems are calculated to validate the OTRT LBE. The results show that OTRT LBE can effectively eliminate the unphysical numerical diffusion induced by the discontinuous heat flux across the phase interface, for one-dimensional to three-dimensional solid-liquid phase change problems.

1. Introduction

Solid–liquid phase change is a common physical phenomenon in nature and relates to many important engineering applications [1–3]. Two key features of solid-liquid phase change problems are: (1) the phase interface, which separates the solid and liquid phases, evolves with time; (2) the phase interface keeps a constant temperature during phase change owing to latent heat. It is challenging to track the phase interface position in advance and couple the phase interface evolution with heat transfer. Moreover, the different thermophysical properties of the solid and liquid phases also increase the difficulty of numerical simulation.

To track the phase interface during solid-liquid phase change, two kinds of equations, which are the phase-field equations [4,5] based on Ginzburg-Landau theory and the energy equations based on energy conservation, have been proposed. In the phase–field equations, the order parameter, which marks the phase distribution and smoothly varies across the diffusive phase interface, is introduced to implicitly track the phase distribution. The temperature field and the phase field are calculated separately. Compared to the phase-field equations, the energy equations are simpler in scheme, therefore have been widely used to simulate solid-liquid phase change. To solve the energy equations, some numerical methods such as finite difference method (FDM) [6,7], control volume method (CVM) [8] and lattice Boltzmann method (LBM) have been proposed.

As an alternative numerical technique, the lattice Boltzmann method (LBM) has drawn increasing attention for its simplicity and efficiency in the simulations of multiphase flow [9–11], conjugate heat transfer [12,13] and solid–liquid phase change. The LBEs for solid–liquid phase change can be classified into two major groups which are: (1) the temperature-based LBEs [14–22] to directly solve the temperature field and (2) the enthalpy-based LBEs [23–29] to solve the enthalpy field then get the temperature field indirectly. In the temperature-based LBEs, the latent heat is considered as a variable heat source term that keeps the temperature of the phase interface constant. Owing to the implicit latent enthalpy term, the heat source term can only be updated by adding some assumptions or a number of iterations, which bring additional numerical error and complexity to the numerical simulations. In addition, all the temperature-based LBEs mentioned above do not consider the difference in heat capacities of the solid and liquid phases. However, the heat capacities of the two phases are generally different and have effect on the heat transfer process before phase change starting.

In the enthalpy-based LBEs, the temperature field is solved indirectly in the form of enthalpy and the phase interface is implicitly tracked by the enthalpy distribution. The corresponding energy governing equation without additional heat source term can be described as [24].

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$$\frac{\partial(\rho c_p T)}{\partial t} = -\nabla\cdot(\rho c_p \vec{u} T) + \nabla\cdot(\lambda\nabla T) - \frac{\partial(\rho L f_L)}{\partial t} - \nabla\cdot(\rho L f_L \vec{u}) \tag{1}$$

where ρ, c_p, T, $\vec{u}$, λ, L, f_L are the density, specific heat, temperature, velocity, thermal conductivity, latent heat of melt and liquid fraction, respectively. $c_p T$ is the sensible enthalpy and $f_L L$ is the latent enthalpy. The convection term $\nabla\cdot(\rho L f_L \vec{u})$, which is induced by the flow of two-phase zone, can be neglected for the isothermal phase change where the two-phase zone acts like solid [2,6,24].

To solve Eq. (1), some enthalpy-based LBEs have been proposed. Chatterjee and Chakraborty [23] developed a hybrid lattice Boltzmann methodology for simulating convection–diffusion transport processes pertinent to melting and solidification problems. The proposed LBE takes compression work and viscosity dissipation into account and considers the latent enthalpy as an additional heat source term. Thus, the implicit latent enthalpy term needs to be calculated via iteration procedure [30]. Another research of Chatterjee [25] is similar. The iteration procedure for enthalpy updating is employed to reduce the difference between the enthalpy predicted by the corresponding evolution equation and the enthalpy dictated by phase-change considerations.

The iteration procedure of updating the latent enthalpy should be removed, because it significantly reduces the computational efficiency. By combining the latent heat source term $\frac{\partial(\rho L f_L)}{\partial t}$ into the transient term $\frac{\partial(\rho c_p T)}{\partial t}$, Huang et al. [24] proposed a new total enthalpy-based LB model. The recovered governing equation is

$$\frac{\partial(\rho H)}{\partial t} = -\nabla\cdot(\rho c_p \vec{u} T) + \nabla\cdot(\lambda\nabla T) \tag{2}$$

where H is the combination of sensible enthalpy $c_p T$ and latent enthalpy $f_L L$, i.e., $H = c_p T + f_L L$. The total enthalpy H is solved by LBE, and then the temperature can be determined by the total enthalpy. Thus, the implicit latent enthalpy term can be eliminated. All the terms in the governing equation, Eq. (2), are explicit now, which makes this model much easier to solve and reduces the numerical error.

Up to now, all the enthalpy-based LBEs mentioned above do not consider the different heat capacities of the solid and liquid phases as well. Recently, Huang and Wu [27] made an important achievement in simulating solid-liquid phase change. They proposed a MRT LBE that can recover Eq. (2) and considers the different heat capacities of the solid and liquid phases. Furthermore, they analyzed the appearance of unphysical numerical diffusion induced by the discontinuous heat flux across the interface in detail, and proved that the unphysical numerical diffusion of two-dimensional melting problems can be eliminated by adjusting the relaxation parameters of D2Q9 MRT model. Following their work, some researchers [26,28] extended the two-dimensional MRT model to three dimensions. Especially, Li and He [28] illustrated how to eliminate the unphysical numerical diffusion of one-phase melting for D3Q7 model in three dimensions.

Obviously, it is not convenient to adjust the relaxation parameters for different D*m*Q*n* MRT models to eliminate the unphysical numerical diffusion. In the present paper, an OTRT LBE is proposed for simulating solid-liquid phase change. By using the Chapman-Enskog expansion, the enthalpy-based energy governing equation can be recovered up to second-order accuracy. Furthermore, detailed theoretical analysis proves that the OTRT LBE can effectively eliminate the unphysical numerical diffusion of arbitrary D*m*Q*n* lattice Boltzmann models for both one-phase and two-phase solid-liquid phase change problems. This feature makes the proposed OTRT LBE flexible to simulate solid-liquid phase change from one dimension to three dimensions. It is equivalent to SRT model in simplicity, but has the same effect as MRT model on eliminating the unphysical numerical diffusion.

The rest part of this paper is organized as follows: the SRT LBE for fluid flow and both the SRT and OTRT LBEs for solid-liquid phase change are introduced in Section 2; Section 3 shows the theoretical analysis of how to eliminate the unphysical numerical simulation by using the OTRT LBE; five test cases are calculated to validate the OTRT LBE in Section 4; finally, conclusions are addressed in Section 5.

2. Lattice Boltzmann equation

2.1. SRT LBE for fluid flow

To solve the enthalpy field, the velocity field needs to be previously calculated. In the present paper, D2Q9 model and D3Q19 model are adopted for simulating two-dimensional and three-dimensional fluid flows, respectively. The SRT LBE for fluid flow with a forcing term can be expressed as [31]

$$f_i(\vec{x} + \vec{e}_i\Delta t, t + \Delta t) - f_i(\vec{x}, t) = -\frac{1}{\tau_f}[f_i(\vec{x}, t) - f_i^{eq}(\vec{x}, t)] + F_i(\vec{x}, t)\Delta t \tag{3}$$

where f_i is the momentum distribution function, f_i^{eq} is the momentum equilibrium distribution function, F_i is the discrete forcing term, τ_f is the relaxation time, t is the lattice simulation time, Δt is the unit time step. The expressions of f_i^{eq} and F_i can be respectively written as

$$f_i^{eq} = w_i\rho\left[1 + \frac{(\vec{e}_i\cdot\vec{u})}{c_s^2} + \frac{\vec{u}\,\vec{u}:(\vec{e}_i\,\vec{e}_i - c_s^2 I)}{2c_s^4}\right] \tag{4}$$

$$F_i(\vec{x}, t) = w_i\left(1 - \frac{1}{2\tau_f}\right)\left[\frac{\vec{e}_i - \vec{u}(\vec{x}, t)}{c_s^2} + \frac{\vec{e}_i\cdot\vec{u}(\vec{x}, t)}{c_s^2}\vec{e}_i\right]\cdot\vec{F}(\vec{x}, t) \tag{5}$$

where w_i is the weight coefficient of direction i, c_s is the lattice sound speed and $\vec{F}$ is the forcing term. The density and velocity are obtained by

$$\rho = \sum_i f_i \tag{6}$$

$$\rho\vec{u} = \sum_i f_i\vec{e}_i + \frac{\vec{F}}{2}\Delta t \tag{7}$$

The relaxation time τ_f is related to the kinematic viscosity through

$$\nu = (\tau_f - 0.5)c_s^2\Delta t \tag{8}$$

The discrete velocities of D2Q9 model and D3Q19 model are respectively given as

$$\vec{e}_i = \begin{bmatrix} 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \end{bmatrix} c \tag{9a}$$

$$\vec{e}_i = \begin{bmatrix} 0 & 1 & -1 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 & 0 & 0 & 1 & -1 & -1 & 1 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \end{bmatrix} c \tag{9b}$$

where c is the lattice speed defined as $c = \Delta x/\Delta t$, and Δx is the unit space step. The corresponding weight coefficients for D2Q9 model and D3Q19 model are respectively given as

$$w_i = \begin{cases} 4/9 & i = 0 \\ 1/9 & i = 1,2,3,4 \\ 1/36 & i = 5,6,7,8 \end{cases} \tag{10a}$$

$$w_i = \begin{cases} 1/3 & i = 0 \\ 1/18 & i = 1 \sim 6 \\ 1/36 & i = 7 \sim 18 \end{cases} \tag{10b}$$

The lattice sound speed c_s is related to the weight coefficient via

$$\sum_{i=0}^{n-1} w_i\vec{e}_{i\alpha}\vec{e}_{i\beta} = c_s^2\delta_{\alpha\beta} \tag{11}$$

where $\delta_{\alpha\beta}$ is the Kronecker Delta function. Its values of D2Q9 model and D3Q19 model are both $1/\sqrt{3}$.

As to the solid–liquid interaction flow, it can be easily simulated