



Investigation of solid-liquid phase change in the spherical capsule using axisymmetric lattice Boltzmann model

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ABSTRACT

The solid-liquid phase change process is important to phase change material (PCM). In this paper, in order to investigate the solid-liquid phase change process in a spherical capsule, the axisymmetric lattice Boltzmann (LB) for phase change is proposed firstly. The problems of one-region phase change in cylindrical coordinate system and solid-liquid phase change by convection in cylindrical enclosure have been solved to verify the present LB model. The distributions of outer wall temperature of spherical capsule are linear. The results show that more heat transferred through the upper region of outer wall may enhance the natural convection and accelerate the process of heat transfer. However, the ratio of energy consumed by latent heat decreases with the slope, leading to more non-uniform temperature distribution. Furthermore, when the slope is larger than 0.2547, more heat is applied to rise the temperature of PCM, resulting in the slower melting rate.

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1. Introduction

The phase change material (PCM) has been widely used in thermal energy storage, temperature maintaining and so on, with the abilities of unobvious temperature variation during solid-liquid phase change process [1]. To reveal the temperature distribution and trace the location of solid-liquid interface, some numerical methods have been proposed, including the conventional computational fluid dynamics (CFD) method [2], molecular dynamics (MD) method [3] and dissipative particle dynamics (DPD) method [4]. Derived from the Boltzmann transport equation, with the abilities of easy parallel computing implementation, the lattice Boltzmann (LB) method has been applied to solve the solid-liquid phase change problems.

There are three categories of phase change LB model [5]: phase-field method, immersed boundary method and enthalpy method. In phase-field method, the order parameter was used to distinguish solid phase and liquid phase by Miller et al. [6,7]. Cartalade et al. [8] proposed a phase-field LB model for 3D crystal growth. Huang and Wu [9] developed a phase change LB model using immersed boundary method, in which the solid-liquid interface was traced by a series of Lagrangian points. However, both the immersed boundary method and phase-field method are complicated [10]. Jiaung et al. [11] developed the enthalpy based phase change LB model. In Jiaung's model, a source term for latent heat was intro-

duced into the evolution equation of temperature distribution function. The temperature and liquid fraction at the same moment were obtained by iterations. Based on this, Huber et al. [12] improved the model and solved the problem of phase change by convection. Then, the model was applied to porous medium (representative elementary volume scale [13–15] and pore scale [16,17]) and nanoparticle-enhanced PCM [18,19]. To avoid the iterations, the implicit scheme [20] and quasi-enthalpy method [21] have been established. Huang et al. [10] formulated a new phase change LB model based on the total enthalpy, and whose accuracy was verified by Luo et al. [22]. Furthermore, the multiple-relaxation-times (MRT) scheme and adaptive mesh refinement scheme were developed by Huang and Wu [5,23]. Wu et al. [24] extended the total enthalpy method to the porous medium. Gao et al. [25,26] established a modified total enthalpy method to avoid the effects of flow field on evolution equation of total enthalpy. In our previous works, the total enthalpy method was employed in phase change under constant heat flux and battery thermal management [27,28].

In this paper, the axisymmetric phase change LB model is firstly proposed. The model is verified by solving the problems of one-region phase change in cylindrical coordinate system and axisymmetric convection dominated phase change. Then, the heat and mass transfer process of phase change in a spherical capsule is investigated. The temperature distributions of capsule's outer wall are linear. The variations of average temperature, temperature standard deviation, total liquid fraction and ratio of energy consumed by latent heat have been considered.

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2. Numerical method

2.1. Conservation equation

The conservation equations, including mass, momentum and energy for incompressible, laminar, Newtonian and pure PCM in cylindrical coordinate are [29]:

$$\nabla \cdot \mathbf{u} = -\frac{u_r}{r} \quad (1)$$

$$\rho \left[\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u}\mathbf{u}) \right] = -\nabla p + \nabla \cdot (\mu \nabla \mathbf{u}) + \frac{\mu}{r} \left(\frac{\partial \mathbf{u}}{\partial r} + \nabla u_r \right) - \frac{\rho \mathbf{u} u_r}{r} - \frac{2\mu \mathbf{u}}{r^2} \delta_r + \mathbf{F} \quad (2)$$

$$\rho \left[\frac{\partial H}{\partial t} + \nabla \cdot (C_p T \mathbf{u}) \right] = \nabla \cdot (\lambda \nabla T) + \frac{\lambda}{r} \frac{\partial T}{\partial r} - \frac{u_r}{r} \rho C_p T \quad (3)$$

where $\nabla = (\frac{\partial}{\partial r}, \frac{\partial}{\partial z})$ is the partial differential operator and $\mathbf{u} = (u_r, u_z)$ is velocity. δ_r is the Kronecker delta with two indices (r coordinate: 1, z coordinate: 0). ρ , p , μ , C_p , T and λ are density, pressure, dynamic viscosity, specific heat at constant pressure, temperature and thermal conductivity, respectively. H in Eq. (3) is the total enthalpy, which can be obtained from:

$$H = C_p T + h_{sl} f_i \quad (4)$$

where h_{sl} and f_i are the latent heat and liquid fraction. \mathbf{F} in Eq. (2) is the body force and in this paper, the buoyancy has been considered. Using the Boussinesq assumption, the buoyancy can be calculated by [10]:

$$\mathbf{F} = -\rho \mathbf{g} \beta (T - T_{ref}) \quad (5)$$

where \mathbf{g} is the acceleration due to gravity. β and T_{ref} are the thermal expansion coefficient and reference temperature.

2.2. Axisymmetric LB model for flow field

The double-distributions model is applied in this paper. The evolution equation for density distribution function (flow field) is as follows [30]:

$$f_i(\mathbf{x} + \mathbf{e}_i \delta t, t + \delta t) = f_i(\mathbf{x}, t) - \chi_f [f_i(\mathbf{x}, t) - f_i^{eq}(\mathbf{x}, t)] + (1 - 0.5\chi_f) \delta t S_i(\mathbf{x}, t) \quad (6)$$

with:

$$\chi_f = \frac{1}{\tau_f} + \left(1 - \frac{1}{2\tau_f}\right) \frac{\delta t e_{ir}}{r} \quad (7)$$

where f_i and f_i^{eq} are the density distribution function and corresponding equilibrium distribution function in direction i . $\mathbf{e}_i = (e_{ir}, e_{iz})$ is the i th discrete velocity. τ_f is dimensionless relaxation time. The equilibrium distribution function can be obtained by [30]:

$$f_i^{eq} = \omega_i \rho \left[1 + \frac{\mathbf{e}_i \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{e}_i \cdot \mathbf{u})^2}{2c_s^4} - \frac{u^2}{2c_s^2} \right] \quad (8)$$

where ω_i is the weight coefficient in direction i , and c_s is the lattice sound speed. In D2Q9 model, the weight coefficient and discrete velocity are given by:

$$\omega_i = \begin{cases} \frac{4}{9} & i = 0 \\ \frac{1}{9} & i = 1, 2, 3, 4 \\ \frac{1}{36} & i = 5, 6, 7, 8 \end{cases} \quad (9)$$

$$\mathbf{e}_i = \begin{cases} (0, 0) & i = 0 \\ c(\cos[\frac{\pi}{2}(i-1)], \sin[\frac{\pi}{2}(i-1)]) & i = 1, 2, 3, 4 \\ \sqrt{2}c(\cos[\frac{\pi}{4}(2i-1)], \sin[\frac{\pi}{4}(2i-1)]) & i = 5, 6, 7, 8 \end{cases} \quad (10)$$

where $c = \Delta x / \Delta t$ is lattice speed and $c_s^2 = 1/3c^2$.

The source term S_i in Eq. (6), can be expressed as:

$$S_i(\mathbf{x}, t) = \left[\frac{1}{\rho c_s^2} (\mathbf{e}_i - \mathbf{u}) \cdot \left(-\frac{2\mu \mathbf{u} \delta_r}{r^2} + \mathbf{F} \right) - \frac{u_r}{r} \right] f_i^{eq} \quad (11)$$

And the macroscopic quantities are given by:

$$\rho = \sum_i f_i - \frac{\delta t}{2} \frac{\rho u_r}{r} \quad (12)$$

$$\rho \mathbf{u} = \sum_i \mathbf{e}_i f_i + \frac{\delta t}{2} \left(\mathbf{F} - \frac{\rho \mathbf{u} u_r}{r} - \frac{2\mu \mathbf{u}}{r^2} \delta_r \right) \quad (13)$$

Using the Chapman-Enskog expansion, Eq. (1) and (2) can be derived from Eq. (6), with [30]:

$$\tau_f = \frac{\mu}{\rho c_s^2 \delta t} + 0.5 = \frac{\nu}{c_s^2 \delta t} + 0.5 \quad (14)$$

where ν is the kinetic viscosity.

2.3. Axisymmetric phase change LB model

Based on the work of Zheng et al. [31] and Huang et al. [10], the evolution equation of total enthalpy distribution function can be developed as follows:

$$g_i(\mathbf{x} + \mathbf{e}_i \delta t, t + \delta t) - g_i(\mathbf{x}, t) = -\frac{1}{2\tau_g} [g_i(\mathbf{x}, t) - g_i^{eq}(\mathbf{x}, t)] + \delta t G_i(\mathbf{x}, t) \quad (15)$$

where g_i and τ_g are the total enthalpy distribution function in direction i and dimensionless relaxation time, respectively. g_i^{eq} is the corresponding equilibrium distribution function, which is obtained from:

$$g_i^{eq} = \begin{cases} rH - rC_p T + \omega_i r C_p T \left(1 - \frac{u^2}{2c_s^2}\right) & i = 0 \\ \omega_i r C_p T \left[1 + \frac{\mathbf{e}_i \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{e}_i \cdot \mathbf{u})^2}{2c_s^4} - \frac{u^2}{2c_s^2}\right] & i \neq 0 \end{cases} \quad (16)$$

The total enthalpy can be calculated from:

$$rH = \sum_i g_i \quad (17)$$

Then, the temperature can be derived from:

$$T = \begin{cases} \frac{H}{C_p} & H < H_s \\ T_s + \frac{H-H_s}{H_l-H_s} (T_l - T_s) & H_s \leq H \leq H_l \\ T_l + \frac{(H-H_l)}{C_p} & H \geq H_l \end{cases} \quad (18)$$

where the subscript “ l ” and “ s ” represent “liquid” and “solid”. The source term in Eq. (15) can be defined as:

$$G_i = \omega_i \frac{\mathbf{e}_i \cdot \mathbf{b}}{c_s^2} \quad (19)$$

$$\mathbf{b} = (b_r, b_z) = \left(\left(1 - \frac{1}{2\tau_g}\right) c_s^2 C_p T, 0 \right) \quad (20)$$

Eq. (3) can be derived from Eq. (15) using the Chapman-Enskog expansion. Firstly, taking a second-order Taylor series expansion to Eq. (15) in time and space, it can be got that:

$$(\partial_t + \mathbf{e}_i \cdot \nabla) g_i + \frac{\delta t}{2} (\partial_t + \mathbf{e}_i \cdot \nabla)^2 g_i = -\frac{1}{\delta t \tau_g} (g_i - g_i^{eq}) + G_i \quad (21)$$

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