An enthalpy-based multiple-relaxation-time lattice Boltzmann method for solid-liquid phase change heat transfer in metal foams

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Abstract

In this paper, an enthalpy-based multiple-relaxation-time (MRT) lattice Boltzmann (LB) method is developed for solid-liquid phase change heat transfer in metal foams under local thermal non-equilibrium (LTNE) condition. The enthalpy-based MRT-LB method consists of three different MRT-LB models: one for the flow field based on the generalized non-Darcy model, and the other two for the PCM and metal foam temperature fields described by the LTNE model. The moving solid-liquid phase interface is implicitly tracked through the liquid fraction, which is simultaneously obtained when the enthalpy-based energy equation of the PCM is solved. The present method has some distinctive features. First, as compared with previous studies, the present method avoids the iteration procedure, thus it retains the inherent merits of the standard LB method and has higher computational efficiency. Second, a volumetric LB scheme instead of the bounce back scheme is employed to realize the nonslip velocity condition in the interface and solid phase regions, which is consistent with the actual situation. Last but not least, reference specific heats have been introduced into the equilibrium moments of the MRT-LB models for the temperature fields, and as a result, the thermal conductivity and specific heat of the PCM (or metal foam) are decoupled. Numerical tests demonstrate that the present method can be
served as an accurate and efficient numerical tool for studying metal foam enhanced solid-liquid phase change heat transfer in latent heat storage. Finally, comparisons are made to offer some insights into the roles of the collision model, volumetric LB scheme and relaxation rate ($\zeta_e$) in the enthalpy-based MRT-LB method.

**Keywords:** Lattice Boltzmann (LB) method; Solid-liquid phase change; Metal foams; Phase change material (PCM); Local thermal non-equilibrium (LTNE) model; Enthalpy method.

1. **Introduction**

Over the past three decades, latent heat storage (LHS) using solid-liquid phase change materials (PCMs) has attracted a great deal of attention because it is of great importance for energy saving, efficient and rational utilization of available resources, and optimum utilization of renewable energies [1-5]. Solid-liquid PCMs absorb or release thermal energy by taking advantage of their latent heat (heat of fusion) during solid to liquid or liquid to solid phase change process. PCMs have many desirable properties, such as high energy storage density, nearly constant phase change temperature, small volume change, etc. However, the available PCMs commonly suffer from low thermal conductivities (in the range of 0.2~0.6 W/(m K)) [1]), which prolong the thermal energy charging and discharging period. In order to overcome this limitation and improve the thermal performance of LHS units/systems, a lot of heat transfer enhancement approaches have been developed, among which embedding PCMs in highly conductive porous materials (e.g., metal foams, expanded graphite) to form composite phase change materials (CPCMs) has long been practiced [6]. High porosity open-cell metal foams, as a kind of promising porous materials with high thermal conductivity, large specific surface area, and attractive stiffness/strength properties, have been widely used for LHS applications [7].
With new experimental techniques and advanced instruments, experimental investigations of heat transfer behaviors in porous systems are becoming more accessible, and the problems of solid-liquid phase change heat transfer in metal-foam-based PCMs have been experimentally studied by many researchers [8-12]. In addition to experimental studies, numerical analyses usually play an important role in studying such problems. In the past two decades, numerical investigations have been extensively conducted to study solid-liquid phase change heat transfer in metal foams [13-23]. These numerical investigations provide valuable design guidelines for practical applications of LHS technologies. Since the thermal conductivity of the metal foam is usually two or three orders of magnitude higher than that of the PCM, the thermal non-equilibrium effect between the PCM and metal foam cannot be neglected. Therefore, the local thermal non-equilibrium (LTNE) model (also called the two-temperature model) has been widely employed for numerical studies [14-23]. However, most of the previous numerical studies [13-20] for solid-liquid phase change heat transfer in metal foams were carried out using conventional numerical methods (mainly finite volume method) based on the discretization of the macroscopic continuum equations. In order to get a thorough understanding of the underlying mechanisms, more fundamental approaches should be developed for solid-liquid phase change heat transfer in metal foams.

The lattice Boltzmann (LB) method [24-28], as a mesoscopic numerical method sitting in the intermediate region between microscopic molecular dynamics method and macroscopic continuum-based methods, has achieved great success in simulating fluid flows and modeling physics in fluids since its emergence in 1988 [29-33]. As highlighted by Succi [34], the LB method should most appropriately be considered not just as a smart Navier-Stokes solver in disguise, but rather like a fully-fledged modeling strategy for a wide range of complex phenomena and processes across scales.
In recent years, the LB method in conjunction with the enthalpy method has been successfully employed to simulate solid-liquid phase change heat transfer in metal foams [21-23]. Gao et al. [21] proposed a thermal LB model to simulate melting process coupled with natural convection in open-cell metal foams under LTNE condition. The influence of foam porosity and pore size on the melting process were investigated and discussed. Subsequently, Gao et al. [22] further developed a thermal LB model for solid-liquid phase change in metal foams under LTNE condition. By appropriately choosing the equilibrium temperature distribution functions and discrete source terms, the energy equations of the PCM and metal foam can be exactly recovered. Most recently, Tao et al. [23] employed an enthalpy-based LB method to study the LHS performance of copper foams/paraffin CPCM. The effects of geometric parameters such as pore density and porosity on PCM melting rate, thermal energy storage capacity and density were investigated.

Up to now, although some progresses have been made in studying solid-liquid phase change heat transfer in metal foams, there are still three key issues remain to be resolved. The first one is to avoid iteration procedure so as to improve the computational efficiency. In previous studies [21-23], the nonlinear latent heat source term accounting for the phase change is treated as a source term in the LB equation of the PCM temperature field, which makes the explicit time-matching LB equation to be implicit. Therefore, an additional iteration procedure is needed at each time step so that the convergent solution of the implicit LB equation can be obtained, which severely affects the computational efficiency, and the inherent merits of the LB method are lost.

The second key issue is to accurately realize the nonslip velocity condition in the interface and solid phase regions. For solid-liquid phase change heat transfer in metal foams, the phase interface is actually a region with a certain thickness because of the interfacial heat transfer between PCM and
Therefore, the phase interface is usually referred as the interface region or mushy zone. Considering the actual situation of the phase change process, it is not appropriate to use the bounce back scheme to impose the nonslip velocity condition in the interface region. This point will be demonstrated in Section 5.2. The third key issue is that the LB models for the temperature fields may suffer from numerical instability because the Prandtl number and the metal foam-to-PCM thermal conductivity ratio are usually very large. In addition, the differences in thermophysical properties (specific heat and thermal conductivity) between liquid and solid PCMs should be taken into account in practical applications.

In the present study, we aim to develop a novel enthalpy-based LB method for solid-liquid phase change heat transfer in metal foams, in which the above-mentioned key issues will be resolved. Considering that the multiple-relaxation-time (MRT) collision model [28] is superior over its Bhatnagar-Gross-Krook (BGK) counterpart [26,27] in simulating solid-liquid phase change heat transfer in metal foams (will be shown in Section 5.1), the MRT collision model is employed in the enthalpy-based LB method. The rest of this paper is organized as follows. The macroscopic governing equations are briefly given in Section 2. Section 3 presents the enthalpy-based MRT-LB method in detail. Section 4 validates the enthalpy-based MRT-LB method. In Section 5, comparisons are made to offer some insights into the present method. Finally, some conclusions are given in Section 6.

2. Macroscopic governing equations

For solid-liquid phase change heat transfer coupled with natural convection in metal foams, to simplify the physical problem, the following assumptions are made: (1) the flow is incompressible and laminar; (2) the thermophysical properties of the metal foam ($m$) and the PCM ($f$) are constant over
the range of temperatures considered, but may be different for the metal foam, liquid PCM (l) and solid PCM (s); (3) the metal foam and the PCM are homogeneous and isotropic, the metal foam/solid PCM are rigid, and the porosity of the metal foam is constant; (4) the volume change during phase change process is neglected, i.e., \( \rho_f = \rho_l = \rho_s \); (5) the thermal dispersion effects and surface tension are neglected.

To take the non-Darcy effect of inertial and viscous forces into consideration, the flow field is described by the generalized non-Darcy model (also called the Brinkman-Forchheimer extended Darcy model) [35-37]. The volume-averaged mass and momentum conservation equations can be written as

\[ \nabla \cdot \mathbf{u} = 0, \quad (1) \]

\[ \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \left( \frac{\mathbf{u}}{\phi} \right) = -\frac{1}{\rho_f} \nabla (\phi p) + v_e \nabla^2 \mathbf{u} + \mathbf{F}, \quad (2) \]

where \( \rho_f \) is the density of the PCM, \( \mathbf{u} \) and \( p \) are the volume-averaged velocity and pressure, respectively, \( \phi \) is the porosity of the metal foam, \( v_e \) is the effective kinematic viscosity, and \( \mathbf{F} \) is the total body force induced by the porous matrix (metal foam) and other external force fields, which can be expressed as [36,37]

\[ \mathbf{F} = -\frac{\phi v_f}{K} \mathbf{u} - \phi \frac{F_d}{\sqrt{K}} \mathbf{u} + \phi \mathbf{G}, \quad (3) \]

where \( K \) is the permeability, \( v_f \) is the kinematic viscosity of the PCM (\( v_f \) is not necessarily the same as \( v_e \)), and \( \mathbf{G} \) is the buoyancy force. The inertial coefficient \( F_d \) (Forchheimer coefficient) and permeability \( K \) depend on the geometry of the metal foam. For flow over a packed bed of particles, based on Ergun’s experimental investigations [38], \( F_d \) and \( K \) can be expressed as [39]

\[ F_d = \frac{1.75}{\sqrt{150\phi}}, \quad K = \frac{\phi d_p^2}{150(1-\phi)^2}, \quad (4) \]

where \( d_p \) is the solid particle diameter (or mean pore diameter). For metal foam with \( \phi = 0.8 \)
considered in the present study, \( F_g \) is set to be 0.068 [15,40].

The LTNE model is employed to take into account the temperature differences between metal foam and PCM. According to Refs. [15,17,20], the energy equations of the PCM (including liquid and solid phases) and the metal foam can be written as follows

\[
\frac{\partial}{\partial t} \left\{ \phi \left[ f_l \rho c_{pl} + (1 - f_l) \rho c_{ps} \right] T_f \right\} + \nabla \cdot (\rho c_{pl} T_f \mathbf{u}) = \nabla \cdot (\phi k_f \nabla T_f) + h_f (T_m - T_f) - \frac{\partial}{\partial t} (\phi \rho L_{mf} f_l),
\]

(5)

\[
\frac{\partial}{\partial t} \left\{ \left( 1 - \phi \right) \rho c_{pm} T_m \right\} = \nabla \cdot \left\{ \left( 1 - \phi \right) k_m \nabla T_m \right\} + h_m (T_f - T_m),
\]

(6)

respectively, where \( T \) is the temperature, \( f_l \) is the fraction of liquid in PCM (\( f_l = 0 \) represents the solid phase, \( f_l = 1 \) represents the liquid phase, and \( 0 < f_l < 1 \) represents the interface region), \( c_r \) is the specific heat, \( k \) is the thermal conductivity, \( h_f = h_{mf} a_{mf} \) is the volumetric heat transfer coefficient (\( h_{mf} \) is the interfacial heat transfer coefficient between PCM and metal foam, \( a_{mf} \) is the specific surface area of the metal foam), and \( L_m \) is the latent heat of phase change. The underlined term in Eq. (5) is the nonlinear latent heat source term accounting for the phase change.

Based on the Boussinesq approximation, the buoyancy force \( \mathbf{G} \) in Eq. (3) is given by

\[
\mathbf{G} = -g \beta (T_f - T_0) f_l,
\]

(7)

where \( g \) is the gravitational acceleration, \( \beta \) is the thermal expansion coefficient, and \( T_0 \) is the reference temperature. The effective thermal conductivities of the PCM and metal foam are defined by

\[
k_{ef} = \phi k_f, \quad k_{em} = (1 - \phi) k_m.
\]

(8)

respectively. The thermal conductivity and specific heat of the PCM are given as follows

\[
k_f = f_l k_l + (1 - f_l) k_s, \quad c_{pf} = f_l c_{pl} + (1 - f_l) c_{ps}.
\]

(9)

In addition to the porosity \( \phi \), solid-liquid phase change heat transfer in metal foams governed by Eqs. (1), (2), (5) and (6) is characterized by the following dimensionless parameters: the Rayleigh number \( Ra \), the Prandtl number \( Pr \), the Darcy number \( Da \), the viscosity ratio \( J \), the metal
foam-to-PCM thermal conductivity ratio $\lambda$, the metal foam-to-PCM thermal diffusivity ratio $\Gamma$, the metal foam-to-PCM heat capacity ratio $\hat{\sigma}$, the dimensionless volumetric heat transfer coefficient (based on pore diameter $d_p$) $H_f$, the Fourier number $Fo$ (dimensionless time), and the Stefan number $St$, which are defined as follows:

$$Ra = \frac{g\beta \Delta T L^3}{v_f \alpha_f}, \quad Pr = \frac{v_f}{\alpha_f}, \quad Da = \frac{K}{L^2}, \quad J = \frac{v_c}{v_f}, \quad \lambda = \frac{k_m}{k_f},$$

$$\Gamma = \frac{\alpha_m}{\alpha_f}, \quad \hat{\sigma} = \frac{(\rho c_r)_m}{(\rho c_r)_f}, \quad H_f = \frac{h_c d_p^2}{k_f}, \quad Fo = \frac{t L^2}{\alpha_f}, \quad St = \frac{c_p \Delta T}{L_n}.$$

where $L$ is the characteristic length, $\Delta T$ is the characteristic temperature, $\alpha_f = k_f / (\rho c_r)_f$ and $\alpha_m = k_m / (\rho c_r)_m$ are thermal diffusivities of the PCM and metal foam, respectively.

Under the local thermal equilibrium (LTE) condition, i.e., $T_f = T_c = T$, the energy equations (5) and (6) can be replaced by the following single energy equation [41]

$$\frac{\partial}{\partial t}(\overline{\rho_f c_r T}) + \nabla \cdot (\rho_f c_r T \mathbf{u}) = \nabla \cdot (k_c \nabla T) - \frac{\partial}{\partial t}(\phi \rho_f L_c f_i),$$

where $\overline{\rho c_r} = \phi [f_r \rho_f c_r + (1-f_r) \rho_c c_m] + (1-\phi) \rho_m c_m$, and $k_c = \phi k_f + (1-\phi) k_m$.

3. Enthalpy-based MRT-LB method

The LB method has been proved to be a promising method for simulating solid-liquid phase change due to its distinctive advantages (see Refs. [33,34] for details). In the LB community, the first attempt to use LB method to study solid-liquid phase change was made by De Fabritiis et al. [42] in 1998. Since then, many LB models for solid-liquid phase change have been developed from different points of view [21-23,43-56]. The existing LB models for solid-liquid phase change mostly fall into one of the following categories: the phase-field method [43-45] and the enthalpy-based method [21-23,46-54]. Additionally, a couple of LB models were recently developed based on some interfacial
tracking methods \cite{55,56}. Owing to its simplicity and effectiveness, the enthalpy-based method plays an increasingly important role in simulating solid-liquid phase change problems.

In what follows, an MRT-LB method in conjunction with the enthalpy method will be presented for solid-liquid phase change heat transfer in metal foams under LTNE condition. The method is constructed in the framework of the triple-distribution-function (TDF) approach: the flow field, the temperature fields of PCM and metal foam are solved separately by three different MRT-LB models.

For two-dimensional (2D) problems considered in the present study, the two-dimensional nine-velocity (D2Q9) lattice is employed. The nine discrete velocities \( \mathbf{e}_i \) of the D2Q9 lattice are given by \cite{27}

\[
\mathbf{e}_i = \begin{cases} (0,0), & i = 0, \\
(\cos[(i-1)\pi/2], \sin[(i-1)\pi/2])c, & i = 1 \sim 4, \\
(\cos[(2i-9)\pi/4], \sin[(2i-9)\pi/4])\sqrt{2}c, & i = 5 \sim 8,
\end{cases}
\]

where \( c = \delta_t / \delta_i \) is the lattice speed with \( \delta_t \) and \( \delta_i \) being the discrete time step and lattice spacing, respectively.

### 3.1 MRT-LB model for the flow field

The MRT method \cite{28,57} is an important extension of the relaxation LB method developed by Higuera et al. \cite{25}. In MRT method, the collision process of the LB equation is executed in moment space, while the streaming process of the LB equation is carried out in velocity space \cite{57}. By using the MRT collision model, the relaxation times of hydrodynamic and non-hydrodynamic moments can be separated. According to Ref. \cite{58}, the MRT-LB equation with an explicit treatment of the forcing term can be written as

\[
f_i^* (\mathbf{x} + \mathbf{e}_i \delta_t, t + \delta_t) = f_i (\mathbf{x}, t) - \tilde{\Lambda}_i \left( f_i - f_i^\alpha \right) \bigg|_{(\mathbf{x},t)} + \delta_i \left( \tilde{\delta}_i - 0.5\tilde{\Lambda}_i \tilde{\delta}_i \right),
\]

where \( f_i (\mathbf{x}, t) \) is the (volume-averaged) density distribution function, \( f_i^\alpha (\mathbf{x}, t) \) is the equilibrium distribution function, \( \tilde{\delta}_i \) is the forcing term, and \( \tilde{\Lambda} = \mathbf{M}_y^\dagger \mathbf{A} \mathbf{M}_y \) is the collision matrix in velocity
space. Here, $M_d$ is the transformation matrix, and $A=\text{diag}\left(s_i,s_i,s_i,s_i,s_i,s_i,s_i\right)$ is the relaxation matrix. The transformation matrix $M_d$ is defined as $M_d=C_dM$, where $M$ is the dimensionless part given by [57]

$$M = \begin{bmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
-4 & -1 & -1 & -1 & 2 & 2 & 2 & 2 & 2 \\
4 & -2 & -2 & -2 & 1 & 1 & 1 & 1 & 1 \\
0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\
0 & -2 & 0 & 2 & 0 & 1 & -1 & -1 & 1 \\
0 & 0 & 1 & 0 & 2 & 1 & 1 & -1 & 1 \\
0 & 0 & -2 & 0 & 2 & 1 & 1 & -1 & 1 \\
0 & 1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 \\
\end{bmatrix}, \quad (13)$$

and $C_d$ is the dimensional part given by

$$C_d=\text{diag}\left(1, c^2, c^4, c, c^3, c, c, c^2, c^3\right). \quad (14)$$

Through the transformation matrix $M_d$, the collision process of the MRT-LB equation (12) can be executed in moment space. Note that $M_d^\dagger\Lambda M_d = M^\dagger\Lambda M$, thus the collision process can be expressed as

$$m^*(x,t) = m(x,t) - A\left(m-m^{\infty}\right)|_{t=\tau} + \delta_i\left(1 - \frac{\Lambda}{2}\right)S. \quad (15)$$

Here, the bold-face symbols $m$, $m^{\infty}$ and $S$ denote 9-dimensional column vectors of moments as follows

$$m = |m\rangle = Mf, \quad m^{\infty} = |m^{\infty}\rangle = Mf^{\infty}, \quad S = |S\rangle = M\hat{S}, \quad (16)$$

where $f = |f\rangle$, $f^{\infty} = |f^{\infty}\rangle$, and $\hat{S} = |\hat{S}\rangle$. For brevity, the Dirac notation $|\rangle$ is employed to represent a 9-dimensional column vector, e.g., $|m\rangle = (m_0, m_1, \ldots, m_9)^\top$. The streaming process is still carried out in velocity space

$$f^\ast_\tau (x+e_\tau, t+\delta_i) = f^\ast_i (x, t), \quad (17)$$

where $f^\ast = M^\dagger m^\ast$. The superscript “$\ast$” denotes that the effect of the solid phase has not yet been considered.
The equilibrium moment \( \mathbf{m}^{eq} \) is defined as \[ \begin{align*}
\mathbf{m}^{eq} &= \rho \left( 1 - 2 + \frac{3|\mathbf{u}|^2}{\phi c^2} \right. \alpha_1 \left. + \frac{\alpha_2}{\phi c^2} \right) \frac{u_x}{c}, \quad \frac{u_y}{c}, \quad \frac{u_z}{c}, \quad \frac{u_x^2 - u_y^2}{\phi c^2}, \quad \frac{u_y u_z}{\phi c^2} \right) ^T,
\end{align*} \] (18)
where \( \rho = \rho_f \) and \( \alpha_1 \) and \( \alpha_2 \) are free parameters. The forcing term in moment space \( \mathbf{S} \) is given by \[ \begin{align*}
\mathbf{S} &= \rho \left( 0, \frac{6 \mathbf{u} \cdot \mathbf{F}}{\phi c^2}, \frac{6 \mathbf{u} \cdot \mathbf{F}}{\phi c^2}, \frac{F_x}{c}, \frac{F_y}{c}, \frac{F_z}{c}, \frac{2(u_x F_y - u_y F_x)}{\phi c^2}, \frac{u_x F_z + u_z F_x}{\phi c^2} \right) ^T,
\end{align*} \] (19)
where \( F_x \) and \( F_y \) are \( x \)- and \( y \)-components of the total body force \( \mathbf{F} \), respectively.

As mentioned in Section 1, it is not appropriate to use the bounce back scheme (liquid fraction \( f_l = 0.5 \) is defined as the phase interface, the collision process (15) is performed for \( f_l > 0.5 \)) [48] to impose the nonslip velocity condition in the interface region. To accurately realize the nonslip velocity condition in the interface and solid phase regions, the volumetric LB scheme [53] is employed in the present study. By using the volumetric LB scheme, the flow field is modeled over the entire domain (including liquid and solid phase regions). Considering the effect of the solid phase, the density distribution function \( f_i \) is redefined as
\[ f_i = f_i^0 + (1 - f_i) f_i^{eq}(\rho, \mathbf{u}), \] (20)
where \( f_i^0 \) is given by Eq. (17), and \( \mathbf{u}_s = 0 \) is the velocity of the solid phase. The above equation is based on a kinetic assumption that the solid phase density distribution function is at equilibrium state [53]. Accordingly, the macroscopic density \( \rho \) and velocity \( \mathbf{u} \) are defined as
\[ \rho = \sum_{i=0}^{\infty} f_i^0, \] (21)
\[ \rho \mathbf{u} = \sum_{i=0}^{\infty} \mathbf{e}_i f_i^0 + \frac{\delta}{2} \rho \mathbf{F}. \] (22)
The macroscopic pressure \( p \) is given by \( p = \rho c_s^2/\phi \). Eq. (22) is a nonlinear equation for the velocity \( \mathbf{u} \) because \( \mathbf{F} \) also contains the velocity. According to Ref. [60], the macroscopic velocity \( \mathbf{u} \) can be
calculated explicitly by
\[ u = \frac{v}{l_0 + \sqrt{l_0^2 + l_1|v|}}, \]  
(23)
where
\[ \rho v = \sum_{i=0}^{8} e_i f_i + \frac{\delta_i}{2} \phi \rho G. \]  
(24)

\[ l_0 = \frac{1}{2} \left( 1 + \phi \frac{\delta_i v_j}{2} \right), \quad l_1 = \phi \frac{\delta_i F \phi}{2 \sqrt{K}}. \]  
(25)

Through the Chapman-Enskog analysis of the MRT-LB equation (12), the mass and momentum conservation equations (1) and (2) can be recovered in the incompressible limit. The effective kinematic viscosity \( v_e \) and the bulk viscosity \( v_b \) are given by
\[ v_e = c_s^2 \left( \frac{1}{s} - \frac{1}{2} \right) \delta, \quad v_b = c_s^2 \left( \frac{1}{s} - \frac{1}{2} \right) \delta, \]  
(26)
respectively, where \( s_{\tau s} = s_v = 1/\tau_v \) (\( \tau_v \) is the relaxation time), \( c_s = c/\sqrt{3} \) is the sound speed of the D2Q9 model.

The equilibrium distribution function \( f_i^{eq} \) in velocity space is given by \( (\alpha_1 = 1, \alpha_2 = -3) \) \[ f_i^{eq} = w_i \rho \left[ 1 + \frac{e_i \cdot u}{c_s^2} + \frac{(e_i \cdot u)^2}{2 \phi c_s^2} - \frac{|u|^2}{2 \phi c_s^2} \right], \]  
(27)
where \( w_0 = 4/9, \quad w_{1-4} = 1/9, \quad \text{and} \quad w_{5-8} = 1/36. \)

3.2 MRT-LB models for the temperature fields

1. Enthalpy-based MRT-LB model

By combining the nonlinear latent heat source term \( \partial_t \left( \phi \rho L_i f_i \right) \) into the transient term in Eq. (5), the following enthalpy-based energy equation of the PCM can be obtained
\[ \frac{\partial H_f}{\partial t} + \nabla \left( \frac{c_p T_f u}{\phi} \right) = \nabla \cdot \left( k_f \frac{T_f}{\rho} \nabla T_f \right) + \frac{h_f \left( T_m - T_f \right)}{\phi \rho}, \]  
(28)
where \( H_f \) is the enthalpy of the PCM. The enthalpy \( H_f \) can be divided into two parts: the sensible
enthalpy $c_pT_f$ and the latent enthalpy $f_iL_a$, i.e.,

$$H_f = c_pT_f + f_iL_a = f_iH_f + (1-f_i)H_s,$$  \hspace{1cm} (29)

$$H_s = c_pT_f,$$  \hspace{1cm} (30)

where $H_f$ is the enthalpy of the liquid PCM, and $H_s$ is the enthalpy of the solid PCM.

For the PCM temperature field governed by Eq. (28), the following MRT-LB equation of the enthalpy distribution function $g_i(x,t)$ is introduced

$$g(x+e\delta_t, t+\delta_t) = g(x, t) - \mathbf{M}^{-1}\mathbf{\Theta}(n_e - n_e^\omega)\big|_{(x,t)} + \delta\mathbf{M}^{-1}\mathbf{S}_{PCM},$$  \hspace{1cm} (31)

where $\mathbf{M}$ is the transformation matrix (see Eq. (13)), and $\mathbf{\Theta} = \text{diag}(\zeta_0, \zeta_2, \zeta_4, \zeta_6, \zeta_8, \zeta_{12}, \zeta_{18}, \zeta_{26})$ is the relaxation matrix. The collision process of the above MRT-LB equation is executed in moment space, i.e.,

$$n_e^*(x,t) = n_e(x,t) - \mathbf{\Theta}(n_e - n_e^\omega)|_{(x,t)} + \delta\mathbf{S}_{PCM},$$  \hspace{1cm} (32)

where $n_e = \mathbf{M}g$ is the moment, and $n_e^\omega = \mathbf{M}g_e^\omega$ is the corresponding equilibrium moment. Here, $g_e^\omega$ is the equilibrium enthalpy distribution function in velocity space. The streaming process is carried out in velocity space

$$g_i(x+e\delta_t, t+\delta_t) = g_i^*(x,t),$$  \hspace{1cm} (33)

where $g^* = \mathbf{M}^{-1}n_e^*$.  

The equilibrium moment $n_e^\omega$ can be chosen as

$$n_e^\omega = \left[H_f, -4H_f + 2c_{f,ref}T_f, 4H_f - 3c_{f,ref}T_f, \frac{c_pT_f}{\phi c}, \frac{c_pT_f}{\phi c}, \frac{c_pT_f}{\phi c}, \frac{c_pT_f}{\phi c}, 0, 0\right]^T,$$  \hspace{1cm} (34)

where $c_{f,ref}$ is a reference specific heat. As did in Ref. [52], the reference specific heat is introduced into the equilibrium moment to make the specific heat and thermal conductivity of the PCM decoupled.

To recover the enthalpy-based energy equation (28), the source term in moment space $\mathbf{S}_{PCM}$ is chosen as
The enthalpy-based energy equation (28) is actually a nonlinear convection-diffusion equation with source term. Therefore, a time derivative term $\frac{1}{2}\delta \hat{\delta}_{,i} S_f$ is incorporated into the source term $S_{PCM}$ as suggested in the literature [61]. Without this derivative term, there must exist an unwanted term $\frac{1}{2}\epsilon \hat{\delta}_{,i} S_f$ in the macroscopic equation recovered from the MRT-LB equation (31). The details will be described later through the Chapman-Enskog analysis.

The enthalpy $H_f$ is computed by

$$H_f = n_{g_i} = \sum_{i=0}^{8} g_{ei}.$$

The relationship between the enthalpy $H_f$ and the temperature $T_f$ is given by

$$T_f = \begin{cases} H_f/c_{\mu}, & H_f \leq H_{\mu}, \\ T_{\beta} + \frac{H_f - H_{\mu}}{H_{\beta} - H_{\mu}} (T_{\beta} - T_{\mu}), & H_{\mu} < H_f < H_{\beta}, \\ T_{\beta} + \frac{(H_f - H_{\beta})/c_{\mu}}, & H_f \geq H_{\beta}, \end{cases}$$

where $H_{\beta} = c_{\mu} T_{\beta}$ is the enthalpy at the solidus temperature $T_{\beta}$, and $H_{\beta} = c_{\mu} T_{\beta} + L_a$ is the enthalpy at the liquidus temperature $T_{\beta}$. The liquid fraction $f_l$ can be determined by

$$f_l = \begin{cases} 0, & H_f \leq H_{\mu}, \\ \frac{H_f - H_{\mu}}{H_{\beta} - H_{\mu}}, & H_{\mu} < H_f < H_{\beta}, \\ 1, & H_f \geq H_{\beta}. \end{cases}$$

The equilibrium enthalpy distribution function $g_{e,ei}$ in velocity space is given by

$$g_{e,ei} = \begin{cases} H_f - \frac{5}{9} c_{f,ae} T_f, & i = 0, \\ w_i c_{ei} T_f \left( \frac{c_{i,ae}}{c_{ei}} + \frac{\epsilon \cdot u}{\phi e_i^2} \right), & i = 1 \sim 8. \end{cases}$$
2. Internal-energy-based MRT-LB model

The energy equation (6) of the metal foam can be rewritten as

$$\frac{\partial}{\partial t} \left( \frac{c_{pm} T_m}{\rho_m} \right) = \nabla \left( \frac{k_m}{\rho_m} \nabla T_m \right) + \frac{h_i (T_f - T_m)}{(1 - \phi) \rho_m}. \quad (41)$$

For the metal foam temperature field governed by the above equation, the MRT-LB equation of the internal-energy distribution function $h_i (x, t)$ is given by

$$h_i (x + e \delta_i + \delta_j) = h_i (x, t) - M^{-1} Q \left( n_i - n_i^e \right) \left|_{(x, \cdot)} \right| + \delta M^{-1} S_{metal}, \quad (42)$$

where $Q = \text{diag} \left( \eta_0, \eta_\nu, \eta_\pi, \eta_\pi, \eta_\phi, \eta_\phi, \eta_\phi, \eta_\phi \right)$ is the relaxation matrix. The collision process of the above MRT-LB equation is executed in moment space, i.e.,

$$n_i^* (x, t) = n_i (x, t) - Q \left( n_i - n_i^e \right) \left|_{(x, \cdot)} \right| + \delta S_{metal}, \quad (43)$$

where $n_i = M h$ is the moment, and $n_i^e = M h^e$ is the corresponding equilibrium moment. Here, $h^e$ is the equilibrium internal-energy distribution function in velocity space. The streaming process is carried out in velocity space

$$h_i (x + e \delta_i + \delta_j) = h_i^* (x, t), \quad (44)$$

where $h^* = M^{-1} n_i^e$. The equilibrium moment $n_i^e$ is defined as

$$n_i^e = \left( c_{pm} T_m, -4 c_{pm} T_m + 2 c_{m,ref} T_m, 4 c_{pm} T_m - 3 c_{m,ref} T_m, 0, 0, 0, 0, 0, 0 \right)^T, \quad (45)$$

where $c_{m,ref}$ is a reference specific heat. The source term in moment space $S_{metal}$ is chosen as

$$S_{metal} = S_{metal} \left( 1, -2, 1, 0, 0, 0, 0, 0, 0 \right)^T, \quad (46)$$

where $S_{metal}$ is given by

$$S_{metal} = S_{ref} + \frac{1}{2} \delta S_{ref} S_{ref}, \quad S_{ref} = \frac{h_i (T_f - T_m)}{(1 - \phi) \rho_m}. \quad (47)$$

The temperature $T_m$ is defined by

$$T_m = \frac{1}{c_{pm}} \sum_{i=0}^{1} h_i. \quad (48)$$
The equilibrium internal-energy distribution function $g_{eq}^{i}$ in velocity space is given by

$$g_{eq}^{i} = \begin{cases} c_{m}T_{m} - \frac{5}{9}c_{m,ref}T_{m}, & i = 0, \\ w_{i}c_{m,ref}T_{m}, & i = 1 - 8. \end{cases}$$  \hspace{1cm} (49)$$

3. Chapman-Enskog analysis

The Chapman-Enskog analysis [63] is employed to derive the macroscopic equations of the MRT-LB equations (31) and (42). To this end, the following multiscale expansions of $n_{x}$, the derivatives of time and space, and the source term are introduced

$$n_{x} = n_{x}^{(0)} + \epsilon n_{x}^{(1)} + \epsilon^{2} n_{x}^{(2)} + \cdots, \quad \partial_{t} = \epsilon \partial_{t}^{(1)} + \epsilon^{2} \partial_{t}^{(2)}, \quad \nabla = \epsilon \nabla_{1}, \quad S_{rf} = \epsilon S_{rf}^{(0)},$$  \hspace{1cm} (50)

where $\epsilon$ ($\epsilon = \delta_{i}$) is a small expansion parameter. Taking a second-order Taylor series expansion to Eq. (31), we can obtain

$$\left(\mathbf{I} \delta_{t}^{(0)} + \mathbf{E} \cdot \nabla_{1}\right)n_{x}^{(0)} + \frac{\delta_{i}}{2} \left(\mathbf{I} \delta_{t}^{(0)} + \mathbf{E} \cdot \nabla_{1}\right)^{2}n_{x}^{(0)} = -\frac{\Theta}{\delta_{t}}\left(n_{x} - n_{x}^{eq}\right) + \hat{S}_{PCM} + \hat{S}_{PCM} + O(\delta_{i}^{3}),$$  \hspace{1cm} (51)

where $\mathbf{E} = (E_{\beta}, E_{\gamma})^T$, in which $E_{\beta} = \mathbf{M}[\text{diag}(e_{\beta,\beta}, e_{\beta,\gamma}, \ldots, e_{\beta,\gamma})]\mathbf{M}^{-1}$ ($\beta = x, y$), and

$$\hat{S}_{PCM} = S_{rf} \left(1, -2, 1, 0, 0, 0, 0, 0, 0, 0\right)^{T},$$  \hspace{1cm} (52)

$$\hat{S}_{PCM} = \frac{1}{2} \delta_{i} \partial_{t} S_{rf} \left(1, -2, 1, 0, 0, 0, 0, 0, 0\right)^{T}. \hspace{1cm} (53)$$

Using the multiscale expansions given by Eq. (50), the following equations in the consecutive orders of $\epsilon$ in moment space can be obtained

$$\epsilon^{0}: \quad n_{x}^{(0)} = n_{x}^{eq},$$  \hspace{1cm} (54)

$$\epsilon^{1}: \quad \left(\mathbf{I} \delta_{t}^{(0)} + \mathbf{E} \cdot \nabla_{1}\right)n_{x}^{(0)} = -\frac{\Theta}{\delta_{t}}n_{x}^{(0)} + \hat{S}_{PCM},$$  \hspace{1cm} (55)

$$\epsilon^{2}: \quad \partial_{t} n_{x}^{(0)} + \left(\mathbf{I} \delta_{t}^{(0)} + \mathbf{E} \cdot \nabla_{1}\right)n_{x}^{(0)} + \frac{\delta_{i}}{2} \left(\mathbf{I} \delta_{t}^{(0)} + \mathbf{E} \cdot \nabla_{1}\right)^{2}n_{x}^{(0)} = -\frac{\Theta}{\delta_{t}}n_{x}^{(2)} + \hat{S}_{PCM}. \hspace{1cm} (56)$$

Using Eq. (55), Eq. (56) can be rewritten as

$$\epsilon^{2}: \quad \partial_{t} n_{x}^{(0)} + \left(\mathbf{I} \delta_{t}^{(0)} + \mathbf{E} \cdot \nabla_{1}\right)\left(1 + \frac{\Theta}{\delta_{t}} n_{x}^{(0)}\right) = \frac{\Theta}{\delta_{t}} n_{x}^{(2)} - \frac{\delta_{i}}{2} \mathbf{E} \cdot \nabla_{1} \hat{S}_{PCM}. \hspace{1cm} (57)$$

Writing out the equations for the conserved moment $n_{x0}$ ($n_{x0} = H_{r}$) of Eqs. (54), (55) and (57), we can obtain
\[
\epsilon^0: \quad n_{e0}^{(0)} = n_{e0}^{\infty}.
\]
\[
\epsilon^1: \quad \partial_{\tau} n_{e0}^{(0)} + c \left[ \partial_{\tau} n_{e0}^{(0)} + \partial_{S} n_{e0}^{(0)} \right] = -\frac{\zeta_0}{\partial_{\tau}} n_{e0}^{(0)} + S_{r_f},
\]
\[
\epsilon^2: \quad \partial_{\tau} n_{s0}^{(0)} + \partial_{S} \left[ \left( 1 - \frac{\zeta_0}{2} \right) n_{s0}^{(0)} + c \nabla_{\tau} \left[ \begin{pmatrix} 1 - \zeta_3/2 & 0 \\ 0 & 1 - \zeta_3/2 \end{pmatrix} \right] n_{s0}^{(0)} \right] = -\frac{\zeta_0}{\partial_{\tau}} n_{s0}^{(2)},
\]

According to Eq. (58), we have
\[
n_{e0}^{(1)} = 0, \quad \forall k \geq 1.
\]

With the aid of Eqs. (58) and (61), we can obtain
\[
\epsilon^1: \quad \partial_{\tau} H_{f} + \nabla_{\tau} \cdot \left( \frac{c_{\tau} T_{f} u}{\phi} \right) = S_{r_f},
\]
\[
\epsilon^2: \quad \partial_{\tau} H_{f} + c \nabla_{\tau} \cdot \left[ \begin{pmatrix} 1 - \zeta_3/2 & 0 \\ 0 & 1 - \zeta_3/2 \end{pmatrix} \right] n_{s0}^{(0)} = 0.
\]

According to Eq. (55), we have
\[
\frac{\zeta_0}{\partial_{\tau}} n_{s0}^{(1)} = \partial_{\tau} n_{s0}^{(3)} + c \left[ \partial_{\tau} n_{s0}^{(3)} + \partial_{S} \left( \frac{3}{2} n_{e0}^{(0)} + \frac{1}{2} n_{s0}^{(0)} + \frac{1}{2} n_{s0}^{(0)} \right) \right]
\]
\[
= -\frac{1}{c} \partial_{\tau} \left( \frac{c_{\tau} T_{f} u}{\phi} \right) + c \nabla_{\tau} \left( \frac{1}{3} c_{f,ref} T_{f} \right),
\]
\[
\frac{\zeta_0}{\partial_{\tau}} n_{s0}^{(1)} = \partial_{\tau} n_{s0}^{(3)} + c \left[ \partial_{\tau} n_{s0}^{(3)} + \partial_{S} \left( \frac{3}{2} n_{e0}^{(0)} + \frac{1}{2} n_{s0}^{(0)} + \frac{1}{2} n_{s0}^{(0)} \right) \right]
\]
\[
= -\frac{1}{c} \partial_{\tau} \left( \frac{c_{\tau} T_{f} u}{\phi} \right) + c \nabla_{\tau} \left( \frac{1}{3} c_{f,ref} T_{f} \right),
\]

Substituting Eqs. (64) and (65) into Eq. (63), the following equation can be obtained
\[
\epsilon^2: \quad \partial_{\tau} H_{f} = \nabla_{\tau} \cdot \left[ \delta_{\tau} \left( \begin{pmatrix} \zeta_3^{-1} & \frac{1}{2} \\ \frac{1}{2} & \zeta_3^{-1} \end{pmatrix} \right) \nabla_{\tau} \left( \frac{c_{\tau} T_{f} u}{\phi} \right) \right] + \frac{c^2}{3} \nabla_{\tau} \left( c_{f,ref} T_{f} \right),
\]

Note that \( \nabla_{\tau} \left( c_{f,ref} T_{f} \right) = c_{f,ref} \nabla_{\tau} T_{f} \), then combining Eqs. (62) and (66) leads to the following macroscopic equation
\[
\frac{\partial H_{f}}{\partial \tau} + \nabla_{\tau} \left( \frac{c_{\tau} T_{f} u}{\phi} \right) = \nabla_{\tau} \cdot \left( \alpha_{f,ref} c_{f,ref} \nabla T_{f} + \delta_{\tau} \left( \zeta_3^{-1} - 0.5 \right) c \partial_{\tau} \left( \frac{c_{\tau} T_{f} u}{\phi} \right) \right) + S_{r_f},
\]
where \( \zeta_3 = \zeta_0 = 1/r_{g} \) (\( r_{g} \) is the relaxation time), and \( \alpha_{f,ref} \) is the reference thermal diffusivity.
\[ \alpha_{f, \text{ref}} = \frac{k_f}{\rho c_p f, \text{ref}} = \varepsilon_h^2 \left( \alpha_{\phi} - \frac{1}{2} \right) \delta_t. \]  

(68)

As compared with Eq. (28), Eq. (67) contains an additional term \( \nabla \left[ \delta \left( \varepsilon_h^{-1} - 0.5 \right) \varepsilon_h \left( c_p f, u / \phi \right) \right] \).

For incompressible thermal flows, the additional term almost has no effect on numerical simulations in most cases. Therefore, the additional term can be neglected, then the enthalpy-based energy equation of the PCM can be recovered from the MRT-LB equation (31). Similarly, the energy equation of the metal foam can be exactly recovered from the MRT-LB equation (42) as

\[ \frac{\partial (c_m T_m)}{\partial t} = \nabla \left( \alpha_{m, \text{ref}} c_{m, \text{ref}} \nabla T_m \right) + S_{m}, \]  

(69)

where \( \alpha_{m, \text{ref}} \) is the reference thermal diffusivity

\[ \alpha_{m, \text{ref}} = \frac{k_m}{\rho c_p m, \text{ref}} = \varepsilon_h^2 \left( \eta_{\phi} - \frac{1}{2} \right) \delta_t, \]  

(70)

where \( \eta_{\phi} = \frac{1}{\tau_{h}} \) (\( \tau_{h} \) is the relaxation time).

In this subsection, the MRT-LB models for the temperature fields have been developed based on the LTNE model. In what follows, some remarks are presented on the proposed models.

**Remark I.** The reference specific heats \( c_{f, \text{ref}} \) and \( c_{m, \text{ref}} \) keep unvaried over the entire domain, which makes the thermal conductivity and specific heat of the PCM (or metal foam) decoupled. As a result, the differences in specific heat and thermal conductivity can be naturally handled (see Eqs. (66) and (67)). According to Eqs. (40) and (49), \( c_{f, \text{ref}} \) and \( c_{m, \text{ref}} \) should satisfy \( c_{f, \text{ref}} < \frac{2}{3} c_{\phi} \) and \( c_{m, \text{ref}} < \frac{2}{3} c_{pm} \), respectively.

**Remark II.** For solid-liquid phase change without convective effect, i.e., the velocity \( u \) is zero, the additional term in Eq. (67) disappears. For solid-liquid phase change coupled with natural convection, the additional term almost has no effect on numerical simulations in most cases, thus it has been neglected in the present study. Theoretically, to remove the additional term, the approaches in
Ref. [53, 61] can be employed.

**Remark III.** The energy equations (28) and (41) are nonlinear convection-diffusion equations with source terms. Therefore, time derivative terms are incorporated into the MRT-LB equations for the temperature fields. Without the derivative terms, there must exist unwanted terms in the macroscopic equations recovered from the MRT-LB equations (31) and (42), as can be seen from Eqs. (55) and (57).

According to Ref. [61], the explicit difference scheme can be used to compute the time derivative terms (e.g., $\partial_t S_{\gamma}$ can be computed by $\partial_t S_{\gamma} = \left[ S_{\gamma}(x, t) - S_{\gamma}(x, t - \delta_t) \right] / \delta_t$), which does not affect the inherent merits of the LB method.

**Remark IV.** The two-dimensional five-velocity (D2Q5) lattice can also be employed. The MRT-LB models for the temperature fields based on D2Q5 lattice are presented in the Appendix.

### 3.3 Boundary conditions and relaxation rates

In this subsection, the boundary conditions and relaxation rates are briefly introduced. For velocity and thermal boundary conditions, the non-equilibrium extrapolation scheme [62] is employed. As did in Ref. [53], the non-slip velocity boundary conditions on the walls are treated based on $f_{i+}$ rather than $f_i$, i.e., they are treated before the consideration of the effect of the solid phase. For a boundary node $x_b$, where $u(x_b, t)$ is known, but $\rho(x_b, t)$ is unknown, the discrete density distribution function $f_{i+}^*(x_b, t)$ at the boundary node $x_b$ is given by

$$f_{i+}^*(x_b, t) = \tilde{f}_{i+}^\alpha(x_b, t) + \left[ f_{i+}^*(x, t) - f_{i+}^\alpha(x, t) \right] \tag{71},$$

where $\tilde{f}_{i+}^\alpha(x_b, t) = f_{i+}^\alpha(\rho(x_b), u(x_b), t)$, and $x_i$ is the nearest neighbor fluid node of $x_b$.

For the flow field, the relaxation rates are set as $s_\rho = s_u = 1$, $s_\rho = s_u = 1.1$, $s_\rho = 1.2$, $s_\rho = 0.5 + v_x / (c_s^2 \delta_t)$ (see Eq. (26)). For the temperature field of the PCM, the relaxation rates are set as $\zeta_0 = 1$, $\zeta_0 = 0.5 + \alpha_{j,ref} / (c_s^2 \delta_t)$ (see Eq. (68)), $\zeta_\alpha = \zeta_{\alpha} = 2 - \zeta_{\alpha}$, $\zeta_{\alpha} = \zeta_{\alpha}$, $\zeta_{\alpha} = 1.2$. For the
temperature field of the metal foam, the relaxation rates are set as \( \eta_0 = 1 \), \( \eta_e = \eta_e = 1.1 \), \( \eta_a = \eta_a = 1.0 \). We would also like to point out that the relaxation rate \( \zeta_e \) plays an important role in simulating solid-liquid phase change heat transfer in metal foams. To reduce the numerical diffusion across the phase interface, we set \( \zeta_e = 2 - \zeta_a \), i.e.,
\[
(\zeta_e^{-1} - 0.5)(\zeta_a^{-1} - 0.5) = 1/4 \quad [52].
\]

4. Numerical tests

In this section, two tests are considered to validate the enthalpy-based MRT-LB method. Some required parameters are set as follows: \( \phi = 0.8 \), \( c_{pl} = c_{pm} = 1 \), \( c_{ps} = c_{pm} = 1 \), \( \dot{\sigma} = 1 \), \( \rho_b = 1 \) (reference density of the PCM), \( c = 1 \) (\( \delta_s = \delta_f = 1 \)). Note that it is no need to restrict \( c = 1 \) in simulations. For simplicity, the volumetric heat transfer coefficient \( (H_v) \) is held constant at 5.9 and the pore size \( (d_p / L) \) is 0.0135. Details about the volumetric heat transfer coefficient and pore size can be found in Refs. [15, 40].

4.1 Solidification by conduction

In this subsection, to validate the MRT-LB models for the temperature fields, conduction-induced solidification in a semi-infinite domain is considered. The schematic diagram of this problem is shown in Fig. 1. The computational domain is filled with metal-foam-based PCM. This problem is symmetrical about \( y = x \). Initially, the PCM is in liquid state at temperature \( T_i \) \( (T_i > T_{melt}) \), here \( T_{melt} \) is the melting temperature. At time \( t = 0 \), the left and bottom walls are lowered to a fixed temperature \( T_c \) \( (T_c < T_{melt}) \), and consequently, solidification begins along the left and bottom surfaces and proceeds into the PCM.

In simulations, the required parameters are chosen as follows: \( \lambda = 10 \), \( St = 4 \), \( T_c = -1 \),
$T_{\text{mel}} = 0$, $T_i = 0.3$, $\Delta T = T_{\text{mel}} - T_i = 1$, $k_f = 0.01$, $c_{f,ref} = 0.5c_{pf}$, and $c_{m,ref} = c_{pm}$. The solidus temperature $T_{p_s} = -0.05$, and the liquidus temperature $T_{p_l} = 0.05$. A grid size of $N_x \times N_y = 200 \times 200$ is employed, and the velocity field is set to be zero ($u = 0$) at each lattice node. In Figs. 2, the phase field at $Fo = 0.02$ is shown. The phase change occurs over a range of temperatures, and the phase interface is usually referred to as the interface region or mushy zone. The liquid fraction distribution, isotherms of the PCM and metal foam at $Fo = 0.02$ are presented in Fig. 3. As shown in the figure, the gaps of the isotherms in the solid phase region are less than those in the liquid phase region because of the release of latent heat on the phase interface. For comparison, the results obtained by the finite difference method (FDM) are also presented in Fig. 3. Obviously, the present results are in good agreement with the FDM results.

![Schematic diagram of 2D conduction-induced solidification in a semi-infinite domain.](image_url)
FIG. 2. Phase field of conduction-induced solidification in a semi-infinite domain at $\text{Fo} = 0.02$.

(a)

(b)

(c)

FIG. 3. The liquid fraction distribution (a), isotherms of the PCM (b) and metal foam (c) at $\text{Fo} = 0.02$.

The blue solid and red dashed lines represent the LBM and FDM results, respectively.
4.2 Melting coupled with natural convection

In this subsection, numerical simulations of melting coupled with natural convection in a square cavity filled with metal-foam-based PCM are carried out to validate the present method. The schematic diagram of this problem is shown in Fig. 4. The distance between the walls is $L$. The horizontal walls are adiabatic, while the left and right walls are kept at constant temperatures $T_h$ and $T_c$ ($T_h > T_c$), respectively. Initially, the PCM is in solid state at temperature $T_i$ ($T_i < T_{meh}$). At time $t = 0$, the temperature of the left wall is raised to $T_h$ ($T_h > T_{meh}$), and consequently, melting begins along the left wall and proceeds into the PCM inside the cavity.

In simulations, the parameters are set as follows: $Da = 10^{-4}$, $Pr = 50$, $F_p = 0.068$, $\lambda = 10^3$, $St = 1$, $J = 1$, $T_h = 1$, $T_{meh} = 0.3$, $T_c = T_i = 0$, $\Delta T = T_h - T_c = 1$, $k_j = 0.0005$, $c_{f,ref} = 0.2c_{pl}$, $c_{m,ref} = c_{pm}$. The solidus temperature $T_{f} = 0.299$, and the liquidus temperature $T_{f} = 0.301$. For $Ra = 10^6$, a grid size of $N_x \times N_y = 150 \times 150$ is employed, and for $Ra = 10^4$, a grid size of $N_x \times N_y = 300 \times 300$ is employed. In Fig. 5, the locations of the phase interface ($f_j = 0.5$) at different Fourier numbers are presented. For comparison, the finite volume method (FVM) solutions reported in
Ref. [15] are also shown in the figure. It can be seen from the figure that the present results agree well with the FVM solutions. From Fig. 5(a) it can be seen that at $Ra = 10^6$, the heat transfer process is dominated by conduction because the metal foam-to-PCM thermal conductivity ratio is very large ($\lambda = 10^3$), and the shape of the phase interface is almost planar during the melting process. As $Ra$ increases to $10^8$, the effect of natural convection on the shape of the phase interface becomes stronger. As shown in Fig. 5(b), due to the convective effect, the phase interface moves faster near the top wall.

FIG. 5. Locations of the phase interface ($f_i = 0.5$) at different Fourier numbers.
As mentioned in Section 1, for solid-liquid phase change in metal-foam-based PCMs, the phase interface is a diffusive interface with a certain thickness rather than a sharp interface, which is usually referred as the interface region or mushy zone. In Fig. 6, the streamlines with the phase interface at different Fourier numbers for $Ra = 10^6$ are shown. From the figure we can see that, during the melting process ($Fo \leq 0.002$), the thickness of the phase interface is around 10 lattices, as a result of the interfacial heat transfer between PCM and metal foam. In the quasi-steady regime ($Fo = 0.008$), the movement of the phase interface is slow enough and it only occupies one or two lattices. The streamlines with the phase interface at different Fourier numbers for $Ra = 10^8$ are shown in Fig. 7. The overall behavior is similar to that with $Ra = 10^6$, albeit with stronger convective effect.
FIG. 6. Streamlines with the phase interface at different Fourier numbers for \( Ra = 10^6 \).

(a) \( Fo = 0.00025 \), (b) \( Fo = 0.001 \), (c) \( Fo = 0.002 \), and (d) \( Fo = 0.008 \).

FIG. 7. Streamlines with the phase interface at different Fourier numbers for \( Ra = 10^8 \).

(a) \( Fo = 0.0004 \), (b) \( Fo = 0.001 \), (c) \( Fo = 0.002 \), and (d) \( Fo = 0.006 \).

The temperature profiles at the mid-height (\( y/L = 0.5 \)) of the cavity at different Fourier numbers for \( Ra = 10^6 \) and \( 10^8 \) are shown in Fig. 8. As can be seen in the figure, the temperature profiles of the PCM and metal foam develop together in a coupled manner. Initially (\( Fo = 0.00005 \)), the metal
foam-to-PCM temperature difference is rather high, but it progressively decreases with the Fourier number. At $\text{Fo} = 0.006$, the temperature profiles of the PCM and metal foam are seen to be nearly identical, which indicates that the thermal non-equilibrium effect between the PCM and metal foam is weak. Fig. 8 clearly shows that the maximum metal foam-to-PCM temperature difference appears near the phase interface. For comparison, the FVM results [15] are also presented in the figure (for clarity, the FVM results at $\text{Fo} = 0.006$ are not presented). It can be observed from the figure that the present results agree well with the FVM results reported in the literature. The variations of the total liquid fraction with the Fourier number for $Ra=10^6$ are shown in Fig. 9. As shown in the figure, the metal foam helps utilize the PCM much more effectively.
FIG. 8. Temperature profiles at the mid-height ($y/L = 0.5$) of the cavity at different Fourier numbers.

FIG. 9. The variations of the total liquid fraction with the Fourier number for $Ra = 10^6$.

5. Comparisons and discussions

In Section 4, the accuracy and effectiveness of the enthalpy-based MRT-LB method have been demonstrated. For melting coupled with natural convection in metal-foam-based PCMs, the fluid flow and heat transfer processes during phase change are rather complicated. In this section, comparisons are made to offer some insights into the roles of the collision model, volumetric LB scheme and relaxation rate ($\zeta_e$) in the present method. All the simulations are carried out with identical initial and boundary conditions at a fixed Rayleigh number $Ra = 10^6$, and the other parameters can be found in Section 4.2.

5.1 MRT vs. BGK

The advantage of MRT collision model over BGK collision model is shown in this subsection. The BGK results denote that the temperature fields are solved by BGK-LB models ($\zeta_i = 1/\tau_s$, $\eta_i = 1/\tau_h$), and the equilibrium distributions are given in Eqs. (40) and (49), while the flow field is still solved by the MRT-LB model presented in Section 3.1. In Fig. 10, the liquid fraction distributions obtained by
BGK and MRT collision models at different Fourier numbers are shown. It is very clear that the phase interface obtained by BGK exhibits significant oscillations (see Fig. 10(a)), which is predominantly due to the numerical diffusion across phase interface. On the contrary, the numerical diffusion across phase interface is almost invisible in the MRT results (see Fig. 10(b)). With additional degrees of freedom, the MRT collision model has the ability to reduce the numerical diffusion across phase interface. In addition, it should be noted that the step-like behavior of the liquid fraction distribution near the liquid/mushy interface (see Fig. 10(b)) is caused by the inevitable numerical error due to the enthalpy formulation.

![BGK](image1)
(a) BGK

![MRT](image2)
(b) MRT

FIG. 10. Local enlargement view of the liquid fraction distributions obtained by BGK (a) and MRT (b) collision models at different Fourier numbers. From left to right: $Fo = 0.001$, $0.002$, and $0.003$.

5.2 Volumetric LB scheme vs. bounce back scheme

In the literature [48], the bounce back scheme was used to impose the nonslip velocity condition
on the phase interface and in the solid phase region. Although this approach has some drawbacks (see Ref. [53] for details), it can produce reasonable results when the phase interface occupies one or two lattices. However, for solid-liquid phase change heat transfer in metal foams, it is not appropriate to use the bounce back scheme to impose the nonslip velocity condition because the phase interface is actually a region (the so-called interface region or mushy zone) with a certain thickness (see Figs. 6 and 7). In what follows, the comparison between the volumetric LB scheme and bounce back scheme is made to demonstrate this point. In Fig. 11, the streamlines at different Fourier numbers are shown. Clearly, significant small-scale (of the order of lattice size) oscillations can be seen in the streamlines obtained by bounce back scheme (see Fig. 11(a)), while the streamlines obtained by volumetric LB scheme are still smooth (see Fig. 11(b)).

FIG. 11. The streamlines obtained by bounce back scheme (a) and volumetric LB scheme (b) at different Fourier numbers. From left to right: \( Fo = 0.001 \), 0.002, and 0.003.
Fig. 12 shows the local enlargement view of the flow fields in the vicinity of interface region obtained by bounce back scheme and volumetric LB scheme at $\text{Fo} = 0.002$. In the flow field obtained by bounce back scheme, nonphysical oscillations occur near the phase interface (marked by the red circles in Fig. 12(a), and note that, $f_i = 0.5$ is defined as the phase interface). On the contrary, the flow field obtained by volumetric LB scheme (see Fig. 12(b)) is rather reasonable. As can be seen in Fig. 12(b), the flow in the interface region is much weaker than that in the liquid phase region near the liquid/mushy interface. It is found that $u_y$ in the liquid phase region near the liquid/mushy interface is of order $O(10^{-3})$, while in the interface region where $f_i = 0.5$, $u_y$ is of order $O(10^{-5})$ or less. In the solid phase region ($f_i = 0$), the velocity is zero ($u = 0$) at each lattice node. Obviously, the flow in the interface region ($0.5 < f_i < 1$) is totally different from that in the liquid phase region. For the phase interface, the following phenomena can be observed. First, the phase interface obtained by bounce back scheme exhibits significant oscillations. Second, as compared with the volumetric LB scheme result, the phase interface obtained by bounce back scheme moves faster near the top wall, but slower near the bottom wall (see top-left and top-right of Fig. 12). From the above comparisons, it can be concluded that the bounce back scheme is not suitable for imposing the nonslip velocity condition in the interface region. Therefore, the volumetric LB scheme [53] is recommended.
5.3 The effect of the relaxation rate \( \zeta_r \)

As shown in Section 5.1, the numerical diffusion across phase interface can be considerably reduced by the MRT collision model with \( \zeta_r = 2 - \zeta_w \). It should be noted that the relaxation rate \( \zeta_r \) has apparent influence on the phase interface. To confirm this statement, numerical simulations are carried out for different values of \( \zeta_r \). In Fig. 13, the local enlargement view of the phase interfaces for different values of \( \zeta_r \) at Fo = 0.002 are presented. Form the figure it can be observed that significant oscillations appear at \( \zeta_r = 1.8 \). As \( \zeta_r \) decreases to 0.1, the numerical diffusion is not apparent, and the phase interface is similar to that at \( \zeta_r = 2 - \zeta_w \). Actually, with the given parameters (see Section 4.2), \( \zeta_r = 0.0296 \) when it is determined by \( \zeta_r = 2 - \zeta_w \). To reduce the numerical diffusion
across phase interface, it is recommended that $\zeta_s = 2 - \zeta_w$.

6. Conclusions

In summary, an enthalpy-based MRT-LB method has been developed for solid-liquid phase change heat transfer in metal foams under LTNE condition. In the method, the moving solid-liquid phase interface is implicitly tracked through the liquid fraction, which is simultaneously obtained when the enthalpy-based energy equation of the PCM is solved by an enthalpy-based MRT-LB model. The present method has three distinctive features. First, the iteration procedure has been avoided, thus it retains the inherent merits of the standard LB method. Second, by using the volumetric LB scheme, the nonslip velocity condition in the interface and solid phase regions can be accurately realized. Moreover, reference specific heats have been introduced into the equilibrium moments of the MRT-LB models for the temperature fields, and then the thermal conductivity and specific heat of the PCM (or metal foam)
are decoupled. As a result, the differences in specific heat and thermal conductivity can be naturally handled, and the relaxation rate related to the thermal conductivity of the PCM (or metal foam) can be appropriately adjusted to improve the numerical accuracy and stability.

Detailed numerical tests of the enthalpy-based MRT-LB method are carried out for two types of solid-liquid phase change heat transfer problems, including the conduction-induced solidification in a semi-infinite domain and melting coupled with natural convection in a square cavity filled with metal-foam-based PCM. It is found that the present results are in good agreement with the FDM/FVM results, which demonstrate that the present method can be served as an accurate and efficient numerical tool for studying metal foam enhanced solid-liquid phase change heat transfer in LHS. Finally, comparisons are made to offer some insights into the roles of the collision model, volumetric LB scheme and relaxation rate (\( \zeta_e \)) in the enthalpy-based MRT-LB method, which are very useful for practical applications.

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Appendix: MRT-LB models for the temperature fields based on D2Q5 lattice

In this Appendix, the MRT-LB models for the temperature fields based on D2Q5 lattice are briefly presented. The five discrete velocities \( \{ \mathbf{e}_i \} \) of the D2Q5 lattice are given by Eq. (11). For the D2Q5 model, the transformation matrix is given by [64]
\[
\begin{bmatrix}
1 & 1 & 1 & 1 & 1 \\
0 & 1 & 0 & -1 & 0 \\
0 & 0 & 1 & 0 & -1 \\
0 & 1 & 1 & 1 & 1 \\
0 & 1 & -1 & 1 & -1
\end{bmatrix}
\]  
\[M = \]

For the enthalpy-based MRT-LB model, the equilibrium moment \( n^e_h \) can be chosen as

\[
n^e_h = \left( H_f, \frac{c_p T_f u_x}{\phi_c}, \frac{c_p T_f u_y}{\phi_c}, \sigma c_{f,ref} T_f, 0 \right)^T, \]

where \( \sigma \in (0,1) \). The source term in moment space is given by \( S_{PCM} = S_{PCM} (1,0,0,\sigma,0)^T \), the relaxation matrix is given by \( \Theta = \text{diag}(\zeta_0,\zeta_x,\zeta_y,\zeta_z,\zeta_v) \), the reference thermal diffusivity is defined as \( \alpha_{f,ref} = c_s^2 (c_s^{-1} - 0.5) \delta_i \), and the equilibrium enthalpy distribution function \( g^e_i \) in velocity space is

\[
g^e_i = \begin{cases} 
H_f - \sigma c_{f,ref} T_f, & i = 0, \\
\frac{1}{4} \sigma c_{f,ref} T_f \left( \frac{c_{f,ref}}{c_{pl}} \right)^2 \frac{\epsilon \cdot u}{\phi_c^2 c_s^2}, & i = 1 \sim 4,
\end{cases}
\]

where \( c_s^2 = c_s^2 \sigma / 2 \) (\( c_s \) is the sound speed of the D2Q5 model).

For the internal-energy-based MRT-LB model, the equilibrium moment \( n^e_i \) can be chosen as

\[
n^e_i = \left( c_p T_m, 0, 0, \sigma c_{n,ref} T_m, 0 \right)^T. \]

The source term in moment space is given by \( S_{metal} = S_{metal} (1,0,0,\sigma,0)^T \), the relaxation matrix is given by \( Q = \text{diag}(\eta_0,\eta_x,\eta_y,\eta_z,\eta_v) \), the reference thermal diffusivity is defined as \( \alpha_{n,ref} = c_s^2 (\eta_s^{-1} - 0.5) \delta_i \), and the equilibrium internal-energy distribution function \( h^e_i \) in velocity space is

\[
h^e_i = \begin{cases} 
c_{n,ref} T_m - \sigma c_{n,ref} T_m, & i = 0, \\
\frac{1}{4} \sigma c_{n,ref} T_m, & i = 1 \sim 4.
\end{cases}
\]

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