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Technical Note

A multicomponent multiphase enthalpy-based lattice Boltzmann method for droplet solidification on cold surface with different wettability

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ABSTRACT

In this paper, a liquid droplet solidification contacting cold solid surface is modeled by a novel multicomponent multiphase enthalpy-based lattice Boltzmann method (LBM). The freezing process of liquid droplet coupled with thermal and mass transfer on cold flat surface with different wettability (θ = 160°, 135°, 60°, 20°) is investigated in detail. The solid volume fraction of droplet solidification with Fourier number are shown under different contact angles. The simulation results show that the solidification time for droplet contacting on a hydrophilic surface is much smaller than that of hydrophobic surface when liquid droplet shares the same initial radius.

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1. Introduction

The solidification process is a common phenomenon in many physical fields, such as air conditioning, phase change energy storage, defrosting, and etc. It is a complicated multiphase flow problem coupled with heat and mass transfer and phase change, especially for multicomponent multiphase system. Over the past several decades, many scientists have studied the liquid-solid phase change process for water droplet either by experimental observation or by macroscopic numerical analysis [1,2]. The LBM has recently gained much attention as a powerful tool to simulate complex physical problem due to advantages of capacity for investigating complicated geometries, simple implementation, high computation efficiency, easy implementation of parallel-processing. It is difficult to determine the phase change interface by conventional computational fluid dynamics (CFD) because of complicated heat and mass transfer mechanism with nonlinear solid-liquid interface characteristics. Three types of liquid-solid phase change LBM models have been developed: immersed boundary method [3], phase-field method [4] and enthalpy-based method [5–13]. Among them, the enthalpy-based LBM model is employed widely due to its simplicity and effectiveness for solid-liquid phase change problem with assumption of no solid-phase movement. Jiaung et al. [5] proposed the enthalpy-based LBM model to simulate phase change problem with heat conduction for the first time. Subsequently, Chatterjee and Chakraborty [6] successfully applied enthalpy updating procedure and one relaxation factor for convergence of iteration. Huber et al. [7] investigated convection-dominated solid-liquid phase change in a cavity by setting number of iterations to be one for calculation efficiency. In this regard, Eshraghi and Felicelli [8] introduced an implicit LBM to handle with the source term, thus avoiding iteration steps. Recently, Huang [9] proposed a new thermal LBM model for solid-liquid phase change by adding latent heat source into transient term, which is characterized by avoiding the iteration process and linear equations.

Since 2015, some research focus on the heat and mass transfer process of solidification for droplets based on enthalpy-based LBM [10–14]. Among them, some [10,11] are applied for single component multiphase system while others [12–14] for multicomponent situations. To the best of knowledge, droplet solidification on cold surface with different wettability using multicomponent multiphase LBM has never been studied. In this paper, the novel multicomponent multiphase enthalpy-based LBM model based on Zhao and Cheng [14] is developed for simulating solidification of a liquid droplet surrounded by air and contacting a cold solid surface.

2. Description of enthalpy-based multicomponent multiphase LBM model

In this section, we briefly present the new enthalpy-based multicomponent multiphase LBM model for liquid-solid phase change.





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The main characteristics for new LBM model are as follows: (1) Triple distribution functions were used, two for velocity field and one for temperature field; (2) Iteration steps and a group of linear equations are avoided by modifying the equilibrium distribution function of the temperature field; (3) The velocity field and temperature field are linked each other through equilibrium function and buoyancy source term; (4) The bounce-back boundary condition for liquid-solid interface is in form of an additional collision term in LBM equation for velocity field.

2.1. Velocity field

The evolution for velocity f_i with immersed moving boundary scheme and force form of exact difference method (EDM) is described as [14]:

$$f_{i}^{k}(x+e_{i}\Delta t,t+\Delta t) = f_{i}^{k}(x,t) - \frac{1-B^{k}}{\tau_{k}}[f_{i}^{k}(x,t) - f_{i}^{k(eq)}(x,t)] + B^{k}\Omega_{i}^{k(s)} + (1-B^{k})\Delta f_{i}^{k}(x,t)$$
(1)

where f_i is the density distribution function at node x and time t, e_i is the discrete velocity in the i direction, k is the component indicator (1 for liquid phase and 2 for gas phase), the D2Q9 discretization scheme for 2D geometry is used in our model,

 τ_k is the relaxation time for component *k*, calculated by:

$$\tau_k = \frac{\upsilon_k}{c_s^2 \Delta t} + \frac{1}{2} \tag{2}$$

where v_k is the kinematic viscosity, c_s is the lattice sound speed equaling to $c/\sqrt{3}$.

 B_k is a weighting function that relates to the dimensionless relaxation time and liquid volume fraction, represented by:

$$B^{k} = \frac{(1 - f_{l})(\tau_{k} - 0.5)}{f_{l} + \tau_{k} - 0.5}$$
(3)

where the liquid fraction f_l is calculated by:

$$f_l = \begin{cases} 0 & H \leqslant H_s \\ \frac{H-H_s}{H_l - H_s}, & H_s < H < H_l \\ 1 & H \ge H_l \end{cases}$$
(4)

with H_s and H_l corresponding to the enthalpies of solidus and liquidus temperature, respectively.

 $f_i^{k(eq)}$ denotes the equilibrium distribution function for the velocity and given by:

$$f_{i}^{k(eq)} = \omega_{i} \rho_{k} \left[1 + \frac{e_{i} \cdot u_{b}}{c_{s}^{2}} + \frac{(e_{i} \cdot u_{b})^{2}}{2c_{s}^{4}} - \frac{u_{b}^{2}}{2c_{s}^{2}} \right]$$
(5)

where w_i is the weighting coefficient, $\Omega_i^{k(s)}$ is an additional collision term bouncing back the non-equilibrium part of the distribution function, represented as:

$$\Omega_{i}^{k(s)} = f_{\bar{i}}^{k}(x,t) - f_{i}^{k}(x,t) + f_{i}^{k(eq)}(\rho_{k},u_{s}) - f_{\bar{i}}^{k(eq)}(\rho_{k},u_{b})$$
(6)

where u_s is the velocity of solid phase and \overline{i} is the opposite direction of *i*.

 Δf_i^k is the force term of EDM proposed by Kupershtokh and Medvedev:

$$\Delta f_i^k(x,t) = f_i^{k(eq)}(\rho_k, u_b + \Delta u_k) - f_i^{k(eq)}(\rho_k, u_b)$$
(7)

where Δu_k is the velocity difference due to total force and can be given as:

$$\Delta u_k = \frac{F_k \Delta t}{\rho_k} \tag{8}$$

where F_k is the total force, composed of three parts, including the particle interaction force F_1^k , the fluid-solid interaction force F_2^k and the gravitational force F_3^k .

The pseudo-potential was applied to represent the particle interaction force:

$$F_{2}^{k} = -\psi_{k}(\rho_{k}(x)) \sum_{x'} \sum_{\bar{k}}^{s} G_{k\bar{k}}(x,x') \psi_{\bar{k}}(\rho_{\bar{k}}(x'))(x'-x)$$
(9)

where $\psi_k(\rho_k(\mathbf{x}))$ is the effective mass, which is a function of the local density. The density value is used for effective mass in this paper for simplicity. k and \bar{k} represent two different fluid components. $G_{kk}(\mathbf{x}, \mathbf{x}')$ is a coupling constant depending on a Green's function.

The fluid-solid interaction force is given by:

$$F_2^k = -\psi_k(\rho_k(x)) \sum_{x'} W(x, x') s(x')(x' - x)$$
(10)

where s(x') is a none-zero constant at the fluid-solid interface and zero otherwise, W(x, x') represents fluid-solid interaction strength and different levels of wettability can be obtained by adjusting the parameter W(x, x').

The macroscopic density, bulk velocity and real physical velocity can be obtained by:

$$\rho_k = \sum_i f_i^k, u_b = \sum_k \rho_k u_k / \sum_k \rho_k, u_r = \sum_k \rho_k u_k + \frac{\Delta t}{2} F_k \tag{11}$$

2.2. Temperature field

The passive scalar method [15] is the extensively applied approach for incorporating thermal effects into LBM, especially for multicomponent multiphase problem. In this work, we adopted the passive scalar method by using single LBM temperature equation.

The evolution equation for temperature field is given by:

$$g_i(x + e_i\Delta t, t + \Delta t) = g_i(x, t) - \frac{1}{\tau_T} [g_i(x, t) - g_i^{eq}(x, t)]$$
(12)

where τ_T is the relaxation time for temperature field which is given below:

$$\tau_T = \frac{\alpha}{c_s^2 \Delta t} + \frac{1}{2} \tag{13}$$

where α is thermal diffusivity and defined as $\alpha = k/(C_p \rho)$ (*k* and C_p are thermal conductivity and specific heat capacity at constant pressure, respectively).

 $g_i^{eq}(x,t)$ is the temperature equilibrium distribution function, given as:

$$g_{i}^{eq} = \begin{cases} H - C_{p}T + \omega_{i}C_{p}T(1 - \frac{u^{2}}{2c_{s}^{2}}) & i = 0\\ \omega_{i}\rho \Big[1 + \frac{e_{i}\cdot u}{c_{s}^{2}} + \frac{(e_{i}\cdot u)^{2}}{2c_{s}^{4}} - \frac{u^{2}}{2c_{s}^{2}} \Big] & i \neq 0 \end{cases}$$
(14)

where *H* is the enthalpy by $H = \sum_{i=1}^{g} B_{i}^{g}$. The temperature can be obtained as follows:

$$T = \begin{cases} T_{s} - \frac{H_{s} - H}{C_{p,s}} & H \leq H_{s} \\ \frac{H_{l} - H}{H_{l} - H_{s}} T_{s} + \frac{H - H_{s}}{H_{l} - H_{s}} T_{l}, & H_{s} < H < H_{l} \\ T_{l} + \frac{H - H_{l}}{C_{p,l}} & H \geq H_{l} \end{cases}$$
(15)

2.3. Computational domain and boundary condition

The 2D computational domain with the size of $N_x \times N_x = 150 \times 150$ in lattice unit is used in this work. One droplet with

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