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Numerical study of convection in phase change material based on Lattice-Boltzmann method

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Abstract. In this paper, the lattice Boltzmann method was studied for the phase change process with convective heat transfer in phase change energy storage materials. Firstly, the macroscopic heat transfer equations for the phase change process with convective heat transfer was given, by which we built the lattice Boltzmann equations for solving the problems. In the model, the speed model of D2Q9 was selected, and the boundary conditions including of non-equilibrium extrapolation and bounce back scheme were selected. Then, the effects of different Rayleigh number on the temperature field and velocity field were analyzed. Further research in a square cavity heat transfer processes with high temperature object and low temperature object were studied, in order to observe the effects of different temperature objects in the phase change process using the changes of phase field.

1. Introduction

Phase change energy storage [1] is a key technology of energy conservation and pollution reduction, with many applications in various fields. In the building energy conservation, phase change material is used to build walls and floor heating to regulate room temperature [2]. In the power peak-loading, the air conditioning and heating system based on PCM have contributed to cut the load [3]. Besides, PCM have been extensively used in solar energy, greenhouses, textiles and thermostat in spacecraft.

Present paper studied the convection in PCM based on Lattice-Boltzmann method, taking relatively stable Double distribution function method and common meshing of D2Q9. The interface of solid and liquid is solved with bouncing format.

2. Governing equations

The convection in phase change divide enthalpy into sensible and latent item, namely. H means total enthalpy, means sensible heat and means latent heat, where. Thus, for the convection equations in phase change [4], under the premise of Boussinesq approximation of incompressible liquid, can be simplified as following:

$$\nabla \bullet \mathbf{u}^{*} = 0 \tag{1}$$

$$\frac{\partial \mathbf{u}^*}{\partial \mathrm{t}^*} + \mathbf{u}^* \bullet (\nabla \mathbf{u}^*) = -\nabla P^* + \Pr \nabla^2 \mathbf{u}^* - \Pr Ra\beta T^* \tag{2}$$

$$\frac{\partial \mathrm{T}^*}{\partial t^*} + \mathbf{u}^* \bullet \nabla T^* = \nabla^2 T^* - \frac{1}{St}\frac{\partial f_l}{\partial t^*} \tag{3}$$

Where

L	—	length
T_1	—	superheat temperature
T_0	—	initial temperature
f_l	—	liquid fraction
C_p	—	specific heat
ν	—	kinematic viscosity
β	—	thermal expansion
g	—	gravity,

The introduction of double distribution and D2Q9 meshing is elaborated in [5, 6], and the velocity $\mathbf{e}_i$ is:

$$\mathbf{e}_i = \begin{cases} (0,0), i = 0 \\ (\cos((i-1)\pi/2), \sin((i-1)\pi/2), i = 1,2,3,4 \\ \sqrt{2}(\cos((2(i-5)+1)\pi/4, \sin((2(i-5)+1)\pi/4), i = 5,6,7,8 \end{cases} \tag{4}$$

Collision equation:

$$f_i(\mathbf{x} + \mathbf{e}_i\Delta t, t + \Delta t) = f_i(\mathbf{x}, t) - \frac{\Delta t}{\tau}(f_i(\mathbf{x}, t) - f_i^{eq}(\mathbf{x}, t)) + \Delta t \times 3w_i g\beta \mathbf{e}_y T(\mathbf{x}, t)\rho(\mathbf{x}, t) \tag{5}$$

$$g_i(\mathbf{x} + \mathbf{e}_i\Delta t, t + \Delta t) = g_i(\mathbf{x}, t) - \frac{\Delta t}{\tau_h}(g_i(\mathbf{x}, t) - g_i^{eq}(\mathbf{x}, t)) \tag{6}$$

Where,

$\omega_0 = 16/36$, $\omega_{\mathrm{i}} = 4/36, (i = 1,2,3,4)$, $\omega_{\mathrm{i}} = 1/36, (i = 5,6,7,8)$, sonic velocity is $\mathrm{c}_s^2 = c^2/3$, pressure p is $\mathrm{P} = \rho c_s^2$, kinetic viscosity $\nu = c_s^2 dt(\tau - 0.5)$,thermal expansion coefficient $\kappa = \mathbf{c}_s^2 dt(\tau_h - 0.5)$.

Static distribution function for f_i:

$$f_i^{eq} = \rho\omega_i\left[1 + 3(\mathbf{e}_i \bullet \mathbf{u}) + \frac{9}{2}(\mathbf{e}_i \bullet \mathbf{u})^2 - \frac{3}{2}\mathbf{u} \bullet \mathbf{u}\right] \tag{7}$$

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Static distribution function for g_i :

$$g_i^{eq} = \mathrm{T}\omega_i\left[1+3(\mathbf{e}_i \bullet \mathbf{u})+\frac{9}{2}(\mathbf{e}_i \bullet \mathbf{u})^2-\frac{3}{2}\mathbf{u}\bullet\mathbf{u}\right] \tag{8}$$

Where, $\mathbf{e}_\mathrm{i}$ and w_i is coefficient, **u** is velocity in macroscope.
Density ρ and momentum $\rho\mathbf{u}$ are defined as:

$$\rho=\sum_{\mathrm{i}=0}^{8} f_\mathrm{i};\ \rho\mathbf{u}=\sum_{i=0}^{8} f_i\mathbf{e}_i \tag{9}$$

Macro temperature is:

$$\mathrm{T}=\sum_{i=0}^{8} g_i \tag{10}$$

Based on non-equilibrium extrapolation, according boundary condition is set up as shown in Fig. 1. Point 3-0-1 lie on the boundary, while 6, 2 and 5 lie in the flow field. Before collision, the distribution function $f_\alpha(O,t)$ needs to be figured out and separated into states of equilibrium and non-equilibrium.

$$f_\alpha(O,t)=f_\alpha^{eq}(O,t)+f_\alpha^{neq}(O,t) \tag{11}$$

The part of equilibrium is obtained through macroscopic quantity of boundary nodes. If node O has unknown macroscopic quantity, then this quantity is replaced by neighbor node's quantity. The distribution function of boundary node O is approximated as:

$$f_\alpha(O,t)=f_\alpha^{eq}(O,t)+[f_\alpha(B,t)-f_\alpha^{eq}(B,t)] \tag{12}$$

Taking collision effect into consideration, the distribution function can be expressed:

$$f_\alpha^{+}(O,t)=f_\alpha^{eq}(O,t)+(1-\frac{1}{\tau})[f_\alpha(B,t)-f_\alpha^{eq}(B,t)] \tag{13}$$

Where, $f_\alpha^{+}(O,t)$ is the distribution function after collision, and τ relaxation time:

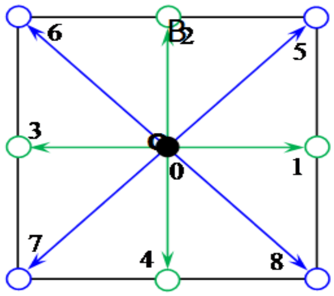

Fig. 1 Non-equilibrium extrapolation scheme

3. Numerical simulation and setup

2-D square is taken as calculation area, investigating different cases of convection in phase change process.

3.1. Convection of right side heated in square

The square's initial temperature is set 200K. Then the left wall is heated, keeping a constant temperature of 400K. The top and bottom walls are adiabatic, taking a set meshing of 64×64. Change Rayleigh number to see the change in melting and convection. The calculation is determined to reach convergence if the error reduces to 10^{-6}. Set Pr=0.02 and St=0.1, see the convection in phase change at Ra=1000, 10000 and 50000.

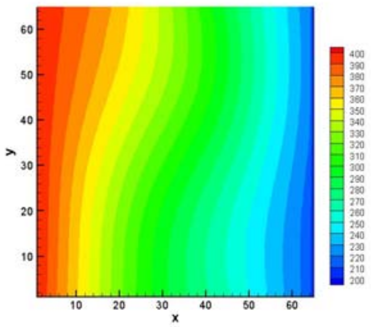

Fig. 2a Temperature field (left) at Ra=1000

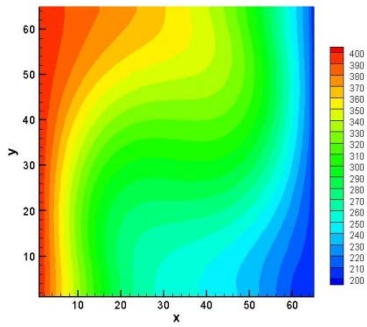

Fig. 2b Temperature field (left) at Ra=10000

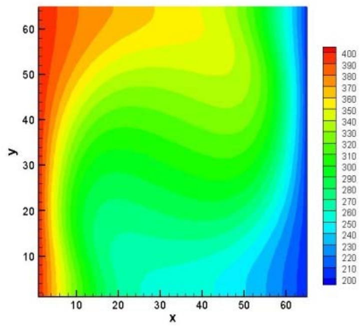

Fig. 2c Temperature field (left) at Ra=50000

When Ra increases, the convection process enhances. And the temperature distribution gets more irregular. The hot liquid moves upwards, transferring some heat to solid to make it melt and leading to collision transfer [7].

Under the same condition, the movement of phase interface with time is shown below (Pr=0.02, St=0.01 and Ra=10000).

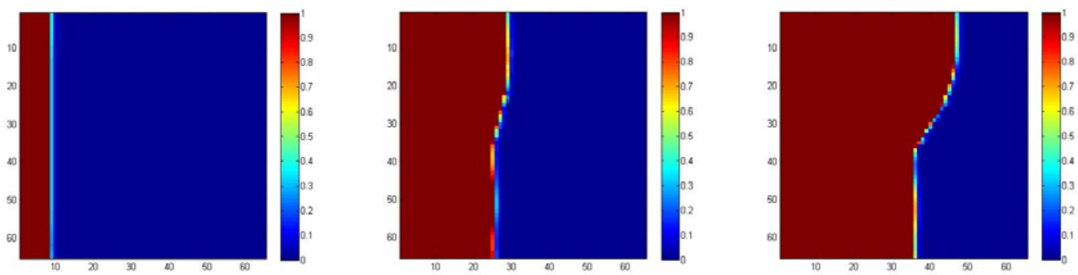

Fig. 3 Trend diagram of phase interface with time

In the initial period, the conduction is dominated compared with convection, leading to a parallel interface to wall. As time goes, the heated liquid moves upwards due to the difference in density. And convection begins to take lead, fasten top part melting.

Keep the parameters constant, and add a constant object of 200K and 400K. Take time point of 23min and 43min.

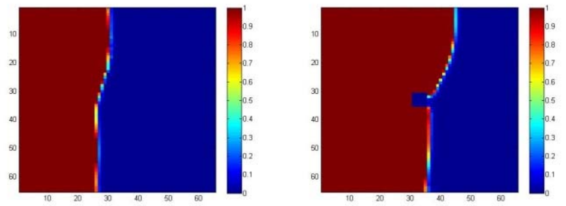

Fig. 4 The phase interface changes with time with low temperature object

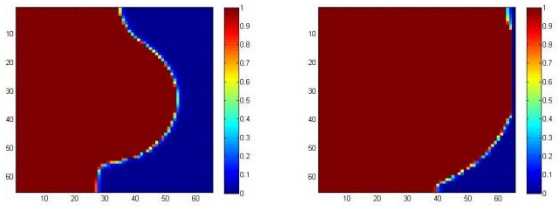

Fig. 5 The phase interface changes with time with high temperature object

As shown in Fig. 4 and 5, the cool object in the square makes little difference, while hot object can make contribute to enhancement of melting to a great extent.

3.2. Convection of bottom side heated in square

All the parameters are set as same as in 3.1. Only change is that the heating boundary is bottom wall [8, 9].

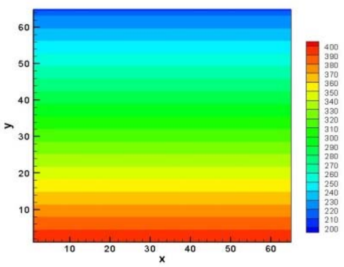

Fig. 6a Temperature field (left) at Ra=1000

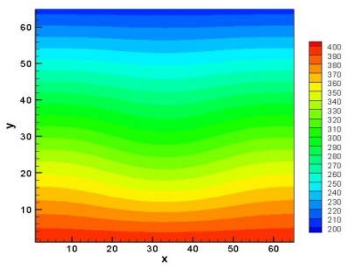

Fig. 6b Temperature field (left) at Ra=10000

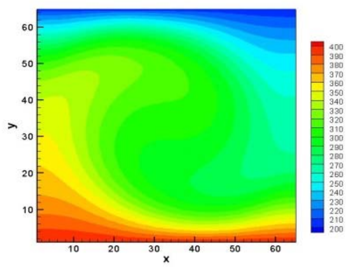

Fig. 6c Temperature field (left) at Ra=50000

With the increase of Ra, convection effect enhances and temperature field changes greatly. Compared to left wall heated, the convection effect is more obvious. It is mainly because the heated liquid upward movement is significant, leading to significant convection effect.

Under the same condition, the movement of phase interface with time is shown below (Pr=0.02, St=0.01 and Ra=10000).

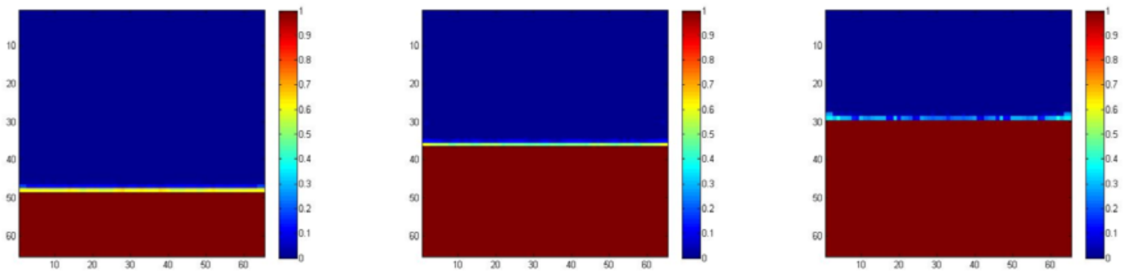

Fig. 7 Trend diagram of phase interface with time

As shown in the figure, in the initial period the conduction is dominated and the interface is parallel to wall. As time goes, the convection begins to take lead. However, due to bottom wall heated, bottom heated liquid all moves upwards, so the interface is still parallel to bottom wall.

Keep other parameters same as previous, insert a cool (200K) and hot (400K) object in the middle. Calculate the movement of phase interface with time, and take time point of 13min and 33min (Pr=0.02, St=0.01, Ra=10000).

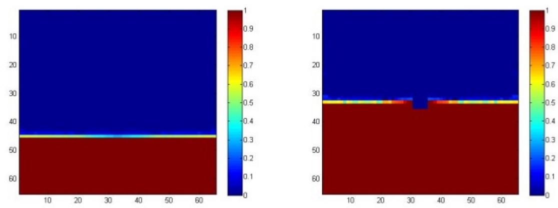

Fig. 8 The phase interface changes with time with low temperature object

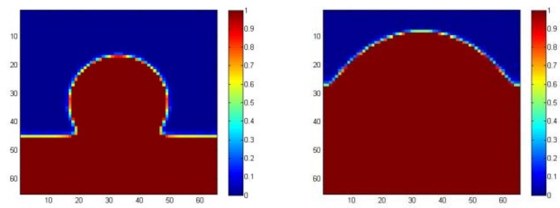

Fig. 9 The phase interface changes with time with high temperature object

As shown above, in the case of cool object in middle, when the interface has not reached the object, the movement of interface is the same as no object. When the interface has reached the object, the other part of interface is not influenced. In the case of hot object, the melting process is fastened obviously.

4. Conclusion

This paper analyzes the melting process of PCM in square based on Lattice-Boltzmann method. Firstly, the convection equations are introduced, and are solved by Lattice-Boltzmann method. Different boundary conditions are studied and according movement of interface is investigated. The thermostatic object is inserted in the middle of square. From the results obtained, we can conclude that when the interface has not reached the cold object, the interface is not influenced. If interface reaches the cold object, the other phase interface is still not influenced. While for the hot object, after reaching the object, the whole melting process is greatly fastened.

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