Comparison of LBM and FVM for Simulation of Solid-Liquid Phase Change Problem with Natural Convection

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Abstract. Phase change materials (PCM) are wildly investigated and used in the fields of thermal energy storage and thermal control of electronics. Numerical simulation is an important method in the research, development, analysis and design of PCM based systems. At present, there are two main numerical methods for the simulation of solid-liquid phase transition problems with natural convection: the finite volume method (FVM) based on macroscopic scale continuity equations, and the lattice Boltzmann method (LBM) based on mesoscopic scale lattice Boltzmann equation. In this paper, the calculation characteristics, speed, efficiency, and accuracy of the two numerical methods are compared, with the classical solid-liquid phase change heat transfer experimental results as benchmark reference. The results obtained in this paper can be used as valuable reference for the selection and use of numerical simulation methods in the study of solid-liquid phase transition problems.

1. Introduction
Phase change materials (PCM) have important application value in the fields of heat storage, cold storage and thermal shock protection of electronics [1]. PCM refer to a class of materials that undergo solid-liquid phase transition by absorbing or releasing a large amount of latent heat at a fixed temperature or in a temperature range. PCM can realize heat storage or release with large capacity under constant temperature, which have advantages of high thermal storage density, compact structure, small heat loss and work stability. PCM can effectively solve the mismatch problem between heat supply and use in time and in order of magnitude in engineering practice, such as solar energy utilization [2], power grid peak load shifting [3-5], energy-efficient building and room temperature regulation, cold-chain logistics [6], the spacecraft thermal control and thermal protection of electronic components [7, 8].

Numerical calculation is an important tool for the study of transportation problems. According to the different of scale, there are mainly three methods for describing and simulating the transportation process: (1) molecular dynamics model at the micro scale; (2) lattice Boltzmann equation at mesoscopic scale; (3) continuity equations at macro scale. The molecular dynamics method tracks the motion state of every molecule, and obtains the macroscopic physical quantity by average through the ensemble. Due to the need to discriminate the molecular scale space and capture the motion within the collision time of molecules, the computation amount is very huge, and the process can only be simulated in a short time and in a small space. Lattice Boltzmann method (LBM) does not need to know the status of each molecule, and just need to obtain the statistical behaviour of molecular
clusters, through simulating the collision and migration process of molecular cluster in mesoscopic scale to reflect the macro-scale diffusion process, such as momentum and energy diffusion, LBM builds the bridge between the micro scale and macro scale. Macroscopic continuity equations, also known as Navier-Stokes equations, mass and energy conservation equations, are governing equations based on the assumption of continuous media and based on the analysis of the micro bodies, finite volume method (FVM) based on the continuity equation is the main method for numerical simulation of macro scale problems.

For the numerical simulation of the flow and heat transfer problem in the solid-liquid phase change process with natural convection, the mainstream methods are the finite volume method FVM based on macroscopic continuity equations, and the lattice Boltzmann method LBM based on mesoscopic scale lattice Boltzmann equations. The two methods have their advantages and characteristics, which have been widely reported in the literature [9-14], while the direct comparison of the two methods is rarely reported. In this paper, the experimental results of the classical convection-type solid-liquid phase transition heat transfer problem are taken as the benchmark reference, and the computation characteristics, calculation speed and accuracy of the two numerical calculation methods (FVM and LBM) will be compared and studied, so as to provide a reference for the selection and use of the numerical calculation method of solid-liquid phase transition problems with natural convection.

2. LBM and FVM model

2.1. Benchmark experiment

Study of the solid-liquid phase transition problem can date back to the 19th century, the Austrian physicist Josef Stefan's study of the formation and evolution of polar ice and the freezing of soil, which calls Stefan problem. Stefan problem is two-phase coupled complex nonlinear problem with moving boundary, and it is generally transient problem, which makes it very difficult to obtain the theoretical solution. Figure 1 shows a typical solid-liquid phase transition process schematically. Supposing that there is a rectangular region of phase change material, the initial state of which is solid. The phase change material is heated from the left boundary, and it is gradually heated and melted. The solid-liquid interface evolves gradually over time, and the whole region is divided into two parts, the region of liquid on the left and the region of solid on the right. In the region of liquid phase, due to the existence of temperature gradient, there will be natural convection, which makes the solid-liquid phase transition problem more complex, from a simple phase change heat conduction problem to a complex problem coupling the natural convection and phase change heat transfer.

![Figure 1. Schematic diagram of the solid-liquid phase transition problem](image_url)

Beckermann and Viskanta [15] studied the melting of Ga in cavity, the thermal properties of which are given in the Table 1. In that experiment, a cavity with length and width of 47.6 mm, depth of 38.1 mm was used. On the left side of the cavity, constant temperature $T_h$ was implemented, which was higher than the melting point of Ga (29.78 °C), on the right cavity side, a constant temperature $T_c$ below its melting point was applied, the rest four faces were kept adiabatic. At the initial time, the
whole phase change material was cooled by the cold wall, which made the whole solid region at a uniform temperature $T_c$. When the left wall was heated by applying high temperature $T_h$, the PCM began to melt, and the liquid-solid interface gradually moved to the right, and finally reached a steady state and formed a stable solid-liquid interface. Five different thermal boundary conditions were studied in the experiment, as shown in Table 2. In this paper, LBM and FVM are used to model and calculate this experiment.

**Table 1. Main thermophysical properties of PCM Ga**

| Parameter                  | Value  |
|----------------------------|--------|
| Melting point $T_m$ (°C)   | 29.78  |
| Latent heat $\Delta H$ (J/kg) | 80160  |
| Solid density $\rho_s$ (kg/m³) | 5903.7 |
| Liquid density $\rho_l$ (kg/m³) | 6094.7 |
| Viscosity $\mu$ (×10⁻³ kg/m·s) | 1.75   |
| Solid specific heat capacity $c_{p,s}$ (J/kg·K) | 372.3  |
| Liquid specific heat capacity $c_{p,l}$ (J/kg·K) | 397.6  |
| Solid thermal conductivity $k_s$ (W/m·K) | 33.49  |
| Liquid thermal conductivity $k_l$ (W/m·K) | 33.68  |
| Expansion coefficient $\beta$ (×10⁻⁴ 1/K) | 1.2    |

**Table 2. Experimental parameters setup**

| Case | $T_h$ (°C) | $T_c$ (°C) | $Ra$ (×10⁵) | $Ste$ (×10⁻²) |
|------|------------|------------|-------------|---------------|
| Case 1 | 40         | 25         | 3.275       | 5.074         |
| Case 2 | 40         | 20         | 3.275       | 5.074         |
| Case 3 | 40         | 10         | 3.275       | 5.074         |
| Case 4 | 35         | 15         | 1.673       | 2.592         |
| Case 5 | 45         | 15         | 4.877       | 7.557         |

**2.2. LBM model**

Here is a brief introduction of the LBM model for convection-type solid-liquid phase transition problems. D2Q9 model is used, both in the momentum and energy field, as shown in Figure 2. The algorithms were programmed in MATLAB by the authors. For brevity, only the evolution equations of flow field and temperature field are given here.

**Figure 2. Diagram of D2Q9 velocity model**

The density evolution equation is

$$f(x + e\Delta t + \Delta t) = f(x, t) - M^{-1} S M[f(x, t) - f^{eq}(x, t)] + \Delta t M^{-1}(I - \frac{S}{2})M \hat{F}$$

(1)

In every computation step, the velocity distribution is calculated first, which is used for the calculation of temperature distribution. The total enthalpy evolution equation is:
\[
g(x + e \Delta t, t + \Delta t) = g(x, t) - M^{-1}S_x M [g(x, t) - g^n(x, t)]
\]  
(2)

For more details about the evolution equation, discrete format, boundary condition algorithms and parameters setting of the model, please refer to our previous work [16].

2.3. FVM model

Enthalpy-porosity model is the most widely adopted model for phase transition problem. Here, we ignore the volume change during phase change, and use Boussinesq approximation to consider the effect of natural convection. The governing equations are provided as follows:

Mass conservation:
\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0
\]  
(3)

Momentum equation
\[
\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = \nabla \cdot (\mu \nabla \mathbf{v}) - \nabla p + \rho \beta (T - T_n) \bar{g}
\]  
(4)

where, in the momentum equation, \( A \mathbf{v} \) is dissipation source term of momentum, which is used to inhibit the velocity in the solid phase and the velocity on solid-liquid interface, according to Darcy’s law, \( A \) is defined in the following form
\[
A = -C (1 - f)^2 \frac{f}{f + \varepsilon}
\]  
(5)

The energy equation based on total enthalpy is
\[
\frac{\partial (\rho H)}{\partial t} + \nabla \cdot (\rho \mathbf{v} H) = \nabla \cdot (k \nabla T)
\]  
(6)

More details about the governing equations, boundary condition settings and numerical calculation parameter settings of enthalpy-porosity method can be found in our previous work [9].

3. Results and discussion

3.1. Model verification by comparing with benchmark experimental results

Figure 3 shows the numerical calculation results of case 1 using LBM and FVM, compared with the corresponding experimental data. Here, the results at the time of 1600 s is selected, when the entire heat transfer process has reached a stable state. It can be seen that in the liquid phase region of the PCM, the temperature presents horizontal distribution, which is the typical characteristic of heat transfer in natural convection problem. In the experimental tests, the temperature at three horizontal lines was monitored. The results were compared, as shown in Figure 3(b). It can be seen that the two were in good agreement. At the same time, we also carried out calculation for the other four experimental conditions and obtained the solid-liquid interface positions at their steady state. The comparison with the experimental results is shown in Figure 4, the two are also in good agreement, indicating that the numerical calculation model built here can well predict the convective melting of PCM. The derivation between the LBM and experimental data is 5.5 %, and the derivation between the FVM and experimental data is 4.9 %, accuracy of the two methods are close to each other, and both of the two are acceptable in practical design.
Figure 3. Verification of the numerical models (comparison with case 1, t=1600 s)

(a) Temperature contour, solid-liquid interface, streamlines in the liquid region; (b) temperature along the three horizontal lines

Figure 4. Locations of liquid-solid interface at steady state under different boundary conditions

3.2. Comparison between LBM and FVM

Table 3 summarizes the hardware configuration and basic parameter settings of the two numerical simulation methods. The computer processor is Intel Core(TM) i7-700 CDU @3.60GHz, the memory capacity is 16.0 GB. LBM is programmed in Matlab, and FVM adopts the commercial software code Fluent. Both methods adopt mesh with size of 100×100, the time step in LBM is 0.0016s, and the time step in FVM is 0.01s, the independence verification of grid and time step are conducted for both of them. For case 1, the total calculation time of LBM is 1.5 hours, and that of FVM is 48 hours. It is not difficult to see that, although the time step of LBM method is about 1/6 of that of FVM method, the calculation time is still much less than that of FVM, which indicates the high efficiency of LBM. The high computational efficiency of LBM benefits from self-programming code, which is generally faster to compute than commercial software packages, and another essential reason lies on the efficiency of the LBM method itself. The lattice Boltzmann equation is an explicit local linear equation, which can be easily numerically calculated, and the pressure can be obtained from the density (equation of gas state), without the need to iteratively calculate the complex Poisson equation of pressure terms as in the Navier-Stokes equation, so the calculation speed is greatly improved.
Table 3. Hardware configuration and the basic parameter settings of the numerical methods

| Numerical method | Hardware configuration | Code | Mesh size | Time step (s) | Computation cost (hour) |
|------------------|------------------------|------|-----------|---------------|------------------------|
| LBM              | Processor: Intel Core i7 with 16 GB RAM | Fluent (Commercial code) | 100×100 | 0.0016 | 1.5 |
| FVM              | Processor: Intel Core i7 with 16 GB RAM | Matlab (programmed by the authors) | 100×100 | 0.01 | 48 |

Figure 5 and Figure 6 visually show the contours of the evolution process of the liquid phase fraction distribution and temperature distribution of the melting process in the cavity in case 1. Both of the two methods can well capture the position of phase interface during the phase transition process. Natural convective flow and heat transfer in liquid phase region are controlled by natural convection vortex. In the early stage of melting (t=100 s), there are three main eddies in the narrow liquid region. The eddies develop over time and fuse into two at 300 s; in the later stage (t=500-1600s), the vortex on the top grows and becomes the main vortex controlling the flow and heat transfer in the whole liquid region.

![Figure 5. Contours of liquid phase fraction in the evolution process](image1)

![Figure 6. Contours of temperature distribution in the evolution process](image2)
To quantitatively compare the computation performance of LBM and FVM, the detailed results of case 1 at steady state is analysed, the velocity along Y direction \( v \) on three horizontal lines (\( Y=0.2, 0.5, 0.8 \)) are compared, as shown in Figure 7. It can be seen that, the two methods get the same variation trend of the velocity distribution, on the left hot wall and right liquid-solid interface, there exists flow boundary layers, the magnitude of which are close, although there exists some minor difference. The main reason for this may be that, at the end of the phase transition process, the flow is strictly unstable, the natural convection changes periodically over time in a small range, such small fluctuation will not significantly influence the heat transfer, so it can be regarded as steady state in view of heat transfer. Due to the difference in the time step size and the difference in numerical calculation models, the two methods shows some differences in capturing this fluctuation.

![Figure 7. Velocity distribution along three horizontal lines](image)

Figure 7. Velocity distribution along three horizontal lines

Figure 8 and Figure 9 quantitatively compare the variation curve of \( Nu \) and \( f \) with dimensionless time \( Ste·Fo \). At the start of melting process, heat conduction dominates the heat transfer, and the heat transfer is strongest when the hot wall surface on the left is in direct contact with the phase change material. Over time, the thickness of the liquid PCM film increases, the thermal resistance increases, and the \( Nu \) number gradually decreases. After \( Ste·Fo \) was larger than 0.05, natural convection gradually strengthens and dominates the heat transfer process. \( Nu \) remains stable and showed periodic changes with the evolution of natural convection vortices. When \( Ste·Fo \) is about 0.3, the melting process tends to be steady, the melting fraction and the position of solid-liquid interface are close to stable state, fluctuation of natural convective vortices gradually tends to be smooth, and the \( Nu \) number also fluctuates within a small range. The results obtained by the two numerical methods are slightly different, but almost agree with each other. In the later melting process (\( Ste·Fo > 0.3 \)), LBM has a good wave capture for the flow heat transfer process, while FVM has a relatively stable result, which may be mainly related to the small time step adopted by LBM.
4. Conclusions
LBM and FVM are the mainstream methods for numerical simulation of the heat transfer process in solid/liquid phase transition problems. The former one has been developed to mature commercial software and has been widely used, with good numerical stability and accuracy. The latter one is being developed rapidly in the past few decades, and corresponding commercial software has not been popularized, and it is mainly developed by self-programming, its most typical features are high computing efficiency and fast speed. The two methods can well capture the dynamic evolution process of solid-liquid interface and natural convective vortex structure and the phase change flow and heat transfer in the phase transition process, and have high computational accuracy and numerical stability, which are in good agreement with the experimental results. When dealing with complex geometric structure problems, FVM's mature geometric and pre-processing software can facilitate modeling and analysis. For the study of regular geometry problems and basic algorithms, LBM's efficient computing performance, strong parallel computing capability, and flexible convenient algorithm modification features show great advantages. In the face of practical problems, the two methods can be selected flexibly according to the needs and existing conditions.
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