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Keywords
boltzmann, lattice, process, two-fluid, simulation, storage, energy, slurry, ice, method, melting

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Abstract

Ice slurry can be used as the thermal storage media in latent cool storage systems for both residential and commercial buildings. This paper presents the investigation of the phase change characteristics of the ice slurry using a two-fluid Lattice Boltzmann Method (TFLBM). The melting and migration processes of the ice slurry are simulated by improving the equilibrium distribution function and matching the relevant parameters such as the kinetic viscosity of ice particle cluster and cross-collision coefficient. The sensitivity analysis of the ice slurry viscosity and cross-collision coefficient are achieved through six numerical experiments, and the ice melting in the internal-melt ice-on-coil thermal storage device is then calculated. The results could be potentially used to guide the design of the ice slurry for cooling both residential and commercial buildings.

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Keywords: Ice storage; Phase change; TFLBM; Numerical simulation

1. Introduction

Over the last two decades, the energy and environment issues have attracted intensive attention. The air-conditioning systems account for a large proportion of total energy consumption worldwide. In order to alleviate this
issue, air-conditioning systems incorporated with cold storage are being considered as a promising solution [1]. Solid-liquid phase change materials (PCMs) can absorb and release a large amount of thermal energy within a small temperature range [2] and are one of the alternative storage media for cold storage systems. As the most commonly used PCMs, ice slurry, which is composed of water and ice particles, has been extensively studied. So far, the thermal storage technology using ice, called ice storage, is generally divided into two types [3]: dynamic storage and static storage. Chaichana [4] developed a computer model to compare energy use in conventional air cooling systems and ice thermal storage systems. Under Thailand electricity tariff rates, the results showed that the ice thermal storage can save energy up to 55%. Koller [5] constructed and experimentally investigated an ice storage unit, which was implemented in the cooling system of an institute building. Long-term measurements of the system showed good in-service behaviours of the ice store. Ruan [6] analyzed the building combined cooling, heating and power (BCHP) plants with an ice storage system, and determined the optimal capacities and operating schedules. However, the ice storage system also brings some difficulties during the preparation, preservation and transportation processes. In practice, the melting and migration always happen because of partially adiabatic tank/tube and density difference between ice particles and water. Thus, optimal design of thermal storage systems for ice slurry requires a thorough understanding of interfacial transport phenomena within the slurry. Because the experimental measurement of interphase interaction in ice slurry is challenging, numerical models with different levels of complexity have been developed and used to analyze such systems [2, 7].

Two traditional methods based on Navier-Stokes equations [8] and molecular dynamics equations [9], are often used in CFD studies. Both methods are differentiated as macroscopic and microscopic schemes, respectively. Eulerian-Eulerian approach or Mixture approach has a high efficiency without an accurate description of the phase interface, while direct numerical simulation (DNS) or molecular dynamics simulation (MDS) requires a significant amount of computational resources [2]. As a powerful alternative to the above two methods, Lattice Boltzmann Method (LBM) bridges the gap between them, which is referred as a mesoscopic scheme. Although LBM is limited by low Mach number (i.e. the velocity is far less than the speed of sound), it is not a key problem in this study as most practical binary mixtures have a slow melting process in real applications [10].

In this paper, the migration and phase transition between water and ice particle cluster are presented. Based on the existing two-fluid Lattice Boltzmann Method (TFLBM) [11], in which cross- and self-collisions are treated independently, TFLBM for a melting ice storage system is developed by improving the equilibrium distribution function and matching the relevant parameters. Sections 2 and 3 describe the TFLBM model and its key parameters, respectively. A sensitivity analysis of collisions terms and numerical simulations of the melting and migration processes are then discussed in the internal-melt ice-on-coil thermal storage device in Section 4. Section 5 provides some conclusions and further development in this direction.

2. The Two-Fluid Lattice Boltzmann Model

The lattice Boltzmann equation was initially derived from the lattice gas automata (LGA) theory. It is also considered as a specially discretized form of the Boltzmann equation in time, space and particular velocity spaces [12]. The popular LBMcs divide the physical region into regular special lattices, and the grid point of the lattice is called lattice site. Microscopic particles are put into each site, where they can only move from one site to its neighboring sites within one computational step (Δt). This movement is often referred to as propagation or streaming.

\[
\begin{align*}
\text{collision:} & \quad f_i(x, t + \Delta t) - f_i(x, t) = \Omega_i \\
\text{streaming:} & \quad f_i(x + c_i \Delta t, t + \Delta t) = f_i(x, t + \Delta t)
\end{align*}
\]  

(1)

where the subscript \(i\) means the predefined propagation directions, \(\Omega_i\) is a collision operator, \(f_i\) represents the probabilities of the distributions in the specified directions \(i\). For the sake of simplicity without loss of generality, the D2Q9 discrete velocity model with two dimensions and nine predefined propagation directions was used in this study.
The TFLBM was developed for simulating the binary mixtures [11]. In comparison with other LBMs, the TFLBM divides the collision operation into three parts, including self-collision term $\Omega_i^{\sigma \sigma}$, cross-collision term $\Omega_i^{\sigma \varsigma}$ and forcing term $F_i^{\sigma}$:

$$\Omega_i^{\sigma} = \Omega_i^{\sigma \sigma} + \Omega_i^{\sigma \varsigma} - F_i^{\sigma} \Delta t$$

(2)

where the superscripts $\sigma$ and $\varsigma$ represent two different components namely water and ice particles respectively, and the superscript $\sigma \varsigma$ means the interaction between the two components. The self-collision term is derived in a similar way as that of the standard LBM [13] which adopts the BGK model, as shown in Eq. (3). For the cross-collision term, the one developed under the isothermal assumption by Luo et al. [14], as expressed in Eq. (4), is used. The derivation of the forcing term $F_i^{\sigma}$ is given in Refs [14, 15].

$$\Omega_i^{\sigma \sigma} = -\frac{1}{\tau_\sigma} \left[ f_i^{\sigma} - f_i^{\sigma(0)} \right]$$

(3)

$$\Omega_i^{\sigma \varsigma} = -\frac{1}{\tau_\varsigma} \rho_\varsigma \frac{f_i^{\sigma(eq)}}{c_s^2} \left( c_i - u \right) \left( u_\sigma - u_\varsigma \right)$$

(4)

$$F_i^{\sigma} = -w_i \rho_\sigma \frac{c_i \cdot a_\sigma}{c_s^2}$$

(5)

where $\rho_\sigma$ and $\rho_\varsigma$ are the macroscopic densities of two components respectively, which can be statistically defined as Eq. (6), $u_\sigma$ and $u_\varsigma$ are the macroscopic velocities of two components respectively, which can be statistically defined as Eq. (7), $\rho$ and $u$ are the total density and velocity of the mixture and can be determined using Eqs. (8) and (9), $c_s$ is the speed of sound whose value is $1/\sqrt{3}$ in lattice unit, $w_i$ is a set of constants dependent on the discrete velocity set $\{c_i\}$, and Eq. (10) gives its formation for D2Q9, $\tau_\sigma$ and $\tau_\varsigma$ are the relaxation time for self-collision and cross-collision respectively, which will be discussed in Section 3, $a_\sigma$ is used as the acceleration term of the fluid $\sigma$. Furthermore, it should be noted that $f_i^{\sigma}$, $f_i^{\sigma(0)}$, $f_i^{\sigma(eq)}$ are the single particle mass density distribution functions, as opposed to the single particle number density distribution functions [11]. The equilibrium distribution function $f_i^{\sigma(0)}$ and $f_i^{\sigma(eq)}$ are given in Eqs. (11) and (12), respectively.

$$\rho_\sigma = \sum_{i=0}^{4} f_i^{\sigma} \quad \text{and} \quad \rho_\varsigma = \sum_{i=0}^{8} f_i^{\varsigma}$$

(6)

$$u_\sigma = \frac{1}{\rho_\sigma} \sum_{i=0}^{4} f_i^{\sigma} c_i \quad \text{and} \quad u_\varsigma = \frac{1}{\rho_\varsigma} \sum_{i=0}^{8} f_i^{\varsigma} c_i$$

(7)

$$\rho = \rho_\sigma + \rho_\varsigma$$

(8)

$$\rho u = \rho_\sigma u_\sigma + \rho_\varsigma u_\varsigma$$

(9)

$$w_i = \begin{cases} 4/9 & i = 0 \\ 1/9 & i = 1, 2, 3, 4 \\ 1/36 & i = 5, 6, 7, 8 \end{cases}$$

(10)
\[ f_{i}^{\sigma(0)} = f_{i}^{\sigma(eq)} \left[ 1 + \frac{1}{c_s^2} (c_i - u) \cdot (u_\sigma - u) \right] \]

\[ f_{i}^{\sigma(eq)} = w_i \rho_\sigma \left[ 1 + \frac{(c_i \cdot u)}{c_s^2} + \frac{(c_i \cdot u)^2}{2c_s^4} - \frac{u^2}{2c_s^4} \right] \]

Note that there is a small difference from the original TFLBM [11]. The last term of \( f_{i}^{\sigma(eq)} \) is only half of the original formation \( -u^2/c_s^2 \). The TFLBM in this study has a better stability and could be perfectly transferred to the standard LBM when the two components have the same parameters. Due to \( \rho_s = \rho_w \) and \( u_s = u_w \) by using Eqs. (8) and (9), respectively. Substituting them into Eqs. (4) and (11), it obtains \( \Omega_{c2} = 0 \) and \( f_i^{\sigma(0)} = f_i^{\sigma(eq)} \). Through combining Eqs. (1)-(12), the TFLBM becomes a standard LBM for a single fluid [16] as follows.

\[ f_{i}^{\sigma} (x + c_i \Delta t, t + \Delta t) = f_{i}^{\sigma} (x, t) - \frac{1}{\tau_\sigma} \left[ f_{i}^{\sigma} (x, t) - f_{i}^{\sigma(eq)} \right] - F_{i}^{\sigma} \Delta t \]

3. Parameters Description of Ice Storage TFLBM

The charging and discharging processes (i.e. freezing and melting of the ice) are critical to ice storage systems. The two most common models used are the heat balance model [17] and enthalpy-porosity model [18]. The heat balance model simulates the heat transfer process in the ice tank without consideration of the specific states of ice particles. In the enthalpy method, the motion of the solid-liquid interface is simulated, but the moving interface introduced the nonlinear behaviour to the phase transition and caused significant computational difficulties in identifying the solution.

One merit of the two-fluid LBM proposed by Luo and Girimaji [11] is that the relaxation time for self- and cross-collision terms are independent, which provides the possibility of introducing the TFLBM to simulate the melting of the ice storage. The self-collision effect is adjusted with the two relaxation scales \( \tau_\sigma \) and \( \tau_\varsigma \), and the different viscosities of the two components can therefore be introduced. The mixture of water and ice is approximated with a miscible mixture, and the miscibility of the mixture can be adjusted easily by changing \( \tau_\sigma \). It is worthwhile to note that it should satisfy the condition of \( \tau_\sigma > 0.5 \) [10], or else it would obtain a nonphysical simulation result.

In this paper, ice is stored in the tank in a form of particle cluster (e.g. ice slurry or snow), and is treated as colloidal dispersions with phase change [19]. Then, the TFLBM is used to simulate the melting and migration processes of ice cluster. There are three assumptions used: a) phase change of ice occurred at a constant temperature of 0°C; b) the energy supplied by the surroundings of the ice storage system is used to melt ice of the interface and; c) the mushy zone of ice is dominated by the diffusion regime [19]. The relaxation time for cross-collision \( \tau_\sigma \) represents diffusion and interaction between water and ice particle cluster. It should be a function of supplied heat \( Q \), the rate of melting \( R \), interaction force between ice and water \( F \), and others, as expressed in Eq. (14).

\[ \tau_\sigma = f(Q, R, F, \cdots) \]

Then, the relaxation time of self-collision \( \tau_\sigma \) can be discussed. From the Chapman-Enskog procedure, the macroscopic equations are derived from TFLBM with the kinetic viscosity as expressed in Eq. (15). The relaxation time for self-collision is controlled by the kinetic viscosity \( \nu_\sigma \). Taking into account the effect of the ice slurry concentration \( \varepsilon \) on the viscosity of the overall fluid, the viscosity of ice particles can be obtained in Eq. (16).

\[ \tau_\sigma = \frac{3}{2} \frac{\Delta t}{Ax^2} \nu_\sigma + \frac{1}{2} \Delta t \]

\[ \nu_\sigma = \frac{1}{\varepsilon} \frac{\Delta t}{Ax^2} \nu_\sigma + \frac{1}{2} \Delta t \]
\[ \nu = (1-\varepsilon)\nu_{\sigma,\text{real}} + \varepsilon \nu_{\varsigma,\text{real}} \]  

(16)

where the subscripts \( \sigma \) and \( \varsigma \) denote water and ice particles, respectively, \( \rho_{\sigma,\text{real}} \) and \( \rho_{\varsigma,\text{real}} \) are the local density of two components, respectively. The multiple relations of the local and average density can be obtained in Eq. (17) based on the volume fraction of ice \( \varepsilon \).

\[ \rho_{\sigma} = (1-\varepsilon)\rho_{\sigma,\text{real}} \quad \text{and} \quad \rho_{\varsigma} = \varepsilon \rho_{\varsigma,\text{real}} \]  

(17)

The Eilers-Chong formula [20], as shown in Eq. (18), is used for the dependence of viscosity on the volume fraction.

\[ \nu(\varepsilon) = \nu_{\sigma} \left[ 1 + \frac{1.25\varepsilon}{1 - \varepsilon/\varepsilon_v} \right] \]  

(18)

where \( \varepsilon_v \) is a parameter to fit with the experimental values of the kinetic viscosity. In this study, it was set as 1. Then, \( \nu(\varepsilon) = \nu_{\sigma} \) if \( \varepsilon = 0 \), while \( \nu(\varepsilon) \rightarrow \infty \) if \( \varepsilon \rightarrow 1 \). This variable viscosity can be introduced to the relaxation time, which was tested by Poiseuille flow with non-constant viscosity \( \nu(y) = \nu_0 + \alpha y \) (See Fig. 1). The analytical solution [19] of the velocity for the Poiseuille flow is given in Eq. (19). The comparison between simulation and analytical results are shown in Fig. 1.

\[ u_y(y) = F_x \frac{(L_y - y)\ln(v_0) + y\ln(v_0 + \alpha L_y) - L_y \ln(v_0 + \alpha y)}{2\alpha \left[ \ln(v_0) - \ln(v_0 + \alpha L_y) \right]} \]  

(19)

where \( \alpha \) is a constant, \( L_y \) is the width of the channel, and \( F_x \) is the external force to drive the flow.

Fig. 1 Velocity profile for a Poiseuille flow with inhomogeneous viscosity.

4. Numerical Simulation and Discussions

Compared to other CFD methods, LBM has advantages such as easy to implement, sympathetic to parallel processing, and capable of handling complex and moving boundaries [16]. In this study, the TFLBM was carried out by a FORTRAN code, and the bounce-back rule [21] was used for all boundaries.
A 2-D test example with honey in a shape of “LBM” [10] was introduced. The honey-like fluid, with the shape of “LBM”, was released from the top of the container filled with water, and flowed down to the bottom of the container due to the gravity. The dissolution process in the test example [10] was reproduced by using the FORTRAN code, which can keep an agreement with daily life experiences of people to the miscible mixtures.

A total of six cases on a 100×100 lattice (Table 1) were designed for sensitivity analysis of kinetic viscosity and interaction effects. In the model of TFLBM, the melting and migration processes of the ice slurry were shown as the variation of density (Fig. 2 and Fig. 3). The starting point of these cases is that snow or ice particle cluster in the shape of “DUT” located at the middle of the storage tank fully filled with water. Then, the ice particle cluster melted at a constant temperature and flowed up due to the buoyancy force. A large value of \( \tau_D \) represents that the tank took in a large quantity of heat and ice melted fast. The parameter of \( \tau_{\text{ice}} \) reflects the compaction degree of ice particle cluster. In this part, the ice floated with the buoyancy force of 0.003 in lattice unit. Unless otherwise indicated, the time step \( \Delta t \) was chosen as 1 (lattice unit) in this work. Fig. 2 presents the 200\(^{\text{th}}\) steps of all cases, in which Fig. 2(a) is the first step (initial state) for these cases. The detailed parameters for each case are given in Table 1.

Table 1 Six cases with different parameters

<table>
<thead>
<tr>
<th>No.</th>
<th>( \tau_D )</th>
<th>( \tau_{\text{water}} )</th>
<th>( \tau_{\text{ice}} )</th>
<th>Remark</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.55</td>
<td>0.6</td>
<td>0.6</td>
<td>Fig. 2(b)</td>
</tr>
<tr>
<td>2</td>
<td>0.55</td>
<td>2.0</td>
<td>0.6</td>
<td>Fig. 2(c)</td>
</tr>
<tr>
<td>3</td>
<td>0.6</td>
<td>10.0</td>
<td>0.6</td>
<td>Fig. 2(d)</td>
</tr>
<tr>
<td>4</td>
<td>0.6</td>
<td>0.6</td>
<td>0.6</td>
<td>Fig. 2(e)</td>
</tr>
<tr>
<td>5</td>
<td>0.75</td>
<td>2.0</td>
<td>10.0</td>
<td>Fig. 2(f)</td>
</tr>
<tr>
<td>6</td>
<td>0.75</td>
<td>2.0</td>
<td>10.0</td>
<td>Fig. 2(g)</td>
</tr>
</tbody>
</table>

Fig. 2 The 200\(^{\text{th}}\) step of each case in Table 1.

By comparing the three pairs of (b) and (e), (c) and (f), (d) and (g), it is easy to see that the size of ice particle cluster with a larger cross-collision coefficient was obviously larger than that of a smaller cross-collision coefficient,
indicating faster melting of ice. These three pairs located at the same height when undergoing the same relaxation time for self-collision. In addition, (b)-(c)-(d) or (e)-(f)-(g) was under the same cross-collision coefficient \( \tau_{D} \), but the relaxation time of ice cluster \( \tau_{ice} \) was higher, which can be seen in Table 1. As the relaxation time is proportional to the kinetic viscosity, a large relaxation time of ice cluster means a large kinetic viscosity. The shapes of ice cluster among these cases ((b)-(c)-(d) or (e)-(f)-(g)) were slightly different, but the difference was much less than those with the cross-collision. This is because the melting effect of the mixture of ice and water is mainly determined by the relaxation time for cross-collision \( \tau_{D} \). It can be seen that the shape of ice cluster was close to the initial shape of “DUT” with an increase of the viscosity of the ice cluster (see Fig. 2(b)-(c)-(d)). It can be concluded that the viscosity of the ice cluster influenced the melting process of the mushy zone to some degree.

Lastly, a 2-D case of the internal melt ice-on-coil storage was studied and the results of the cross-section of the tank are shown in Fig. 3. The parameters used in this case are: \( \tau_{D}=1.0, \tau_{water}=1.0, \tau_{ice}=6.0 \) and the gravity force constant is -0.001. At the beginning of the simulation, the tank was filled with the ice slurry except that the circle tube was filled with water. Due to the energy introduced by the tube, the ice slurry was melted and transferred to water. It can be observed that the melting process of ice slurry was concentric cylinder without gravity, as shown in Fig. 3(a)-(d). When the gravity is considered, the water outside the tube generated by the melting of ice slurry slowly accumulated at the bottom of the tank, which can be clearly seen in Fig. 3 (e)-(h). This phenomenon agreed well with the melting process qualitatively in our daily life, such as liquid water flow and snow melting processes in a snowpack [22].

Fig. 3 The internal melt ice storage with or without gravity. The flames (a)-(d) consider zero gravity and (e)-(h) consider a gravity force constant of -0.001.

5. Conclusions and Future Work

In this paper, the TFLBM for melting ice storage system was developed using improved equilibrium distribution function and the relevant parameters. The cross-collision was used to reflect the melting of ice particles and the diffusion between water and ice particle cluster in the mushy zone, while the self-collision term was associated with the viscosity of water or ice cluster.

The TFLBM was applied to simulate the melting and migration processes of ice slurry in a tank by adding the non-constant viscosity, which was dependent on the volume fraction of the ice particle cluster. The sensitivity

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analysis of the viscosity and cross-collision coefficient showed that the melting of the ice cluster was mainly governed by the relaxation time for cross-collision, and the deformation behaviour and migratory ability of the ice cluster are mainly affected by its viscosity.

Compared to other CFD methods, LBM has the advantages of sympathetic to parallel processing. In the next step, the acceleration implementations of parallel processing on GPU will be explored. Furthermore, the detailed function relationship of the cross-collision coefficient and its applicability in other latent cool storage systems need to be further studied.

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