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### Research paper

# Lattice Boltzmann simulation of convection melting in complex heat storage systems filled with phase change materials



Kang Luo, Feng-Ju Yao, Hong-Liang Yi\*, He-Ping Tan\*

School of Energy Science and Engineering, Harbin Institute of Technology, Harbin 150001, PR China

#### HIGHLIGHTS

- Convection melting in multitube heat storage systems are numerical studied by LBM.
- Different lattice Boltzmann models for phase change are systematically compared.
- The influences of various numbers and arrangements of tubes are investigated.
- Effects of Rayleigh and Stefan numbers on volume melt fraction of PCM are examined.

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#### ABSTRACT

In the present study, a double-population lattice Boltzmann method is applied to the simulation of convection—diffusion phenomena associated with solid—liquid phase transition processes. The research focus is the advancement of the lattice Boltzmann method to complex multitube heat storage system with different numbers and arrangements of tubes. Firstly, a systematic comparison of different lattice Boltzmann models for thermal and flow field in the phase change process is numerically conducted in a square cavity, and the numerical results are validated by the literature data. Then, a comprehensive analysis has been performed in order to investigate the influence of various numbers and arrangements of tubes on the melting dynamics of shell and tube models with different Rayleigh and Stefan numbers. The computational results show how the transient phase-change process, expressed in terms of the volume melt fraction of phase change materials (PCM), depends on the thermal and geometrical parameters of the system.

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#### 1. Introduction

The fundamental of heat transfer and flow in phase change materials (PCM) has received considerable attention during the past two decades due to its potential for thermal energy storage systems. There exists a wide range of applications for such systems [1–3], such as energy storage in buildings, electronics cooling, material processing and thermal management of spacecraft. Theoretical, numerical and experimental studies in the field have yielded extensive literature on various aspects of the phase-change problems, including basic studies of phase-change phenomena [4],

material properties [5], experimental methods and heat transfer enhancement [6–8], mathematical modeling and numerical techniques [9–11]. Among them, numerical simulation is a major focus for its economy and high efficiency, which can significantly improve the understanding of convection melting processes in heat storage systems. It is concluded in the critical review of Agyenim et al. [7] that the most common numerical approach has been the use of enthalpy formulation.

Some well-developed methods have been applied to simulate the convection melting models, such as finite difference method (FDM) [12], finite volume techniques (FVM) [13,14], finite element method (FEM) [15] and lattice Boltzmann method (LBM) [16]. These numerical simulations are mainly based on two types of grid systems, namely, fixed grid [17] and adaptive grid [18], in which, the enthalpy-based LBM is a newly introduced fixed grid based approach for phase change problems.

<sup>\*</sup> Corresponding authors. Tel.: +86 451 86412674.

E-mail addresses: yihongliang@hit.edu.cn (H.-L. Yi), tanheping@hit.edu.cn (H.-P. Tan).

Nomenclature		Ra	Rayleigh number, $g\beta\Delta Tl^3/\nu\chi$	
C	specific heat kU/(kg V)	<b>S</b>	diagonal matrix of non-negative relaxation rates	
$C_p$	specific heat, kJ/(kg K)	$S_t$	Stefan number, $C_p\Delta T/L$	
c	lattice speed, m/s	$T \\ T^*$	temperature, K	
e	propagation velocity in the lattice, m/s	•	dimensionless temperature	
F	Buoyancy, (kg m)/s <sup>2</sup>	u	macroscopic velocity vector, m/s	
$F_o$	Fourier number, $\chi t/l^2$	w	weight function	
f	external body forces per unit mass, particle			
_	distribution function for velocity field	Greek symbols		
$f_l$	volume fraction of liquid	β	thermal expansion coefficient, 1/K	
g	the acceleration due to gravity, m/s <sup>2</sup>	ho	density, kg/m <sup>3</sup>	
g	particle distribution function for thermal field	$ au_{ u}$ , $ au_{T}$	relaxation time for velocity and temperature fields	
Н	total enthalpy, kJ/kg	$\mu$	dynamic viscosity, kg/(m s)	
$H_l$	enthalpy of the liquid phase at the melting	ν	kinematic viscosity, m <sup>2</sup> /s	
	temperature, kJ/kg	χ	thermal diffusivity, m <sup>2</sup> /s	
$H_s$	enthalpy of the solid phase at the melting temperature,	Δ	fraction of an intersected link of curved wall in the	
	kJ/kg		fluid region	
k	thermal conductivity, W/(m K)	$\Delta T$	Temperature difference, $T_h - T_c$	
L	latent heat of melt, kJ/kg	$\Omega$	collision operator	
l	characteristic length, m			
M	the transformation matrix	Subscri	Subscripts	
m	velocity moments of $f$	ave	average	
Nu	Nusselt number, $ql/k\Delta T$	eq	equilibrium distribution	
Nu <sub>ave</sub>	average Nusselt number	h, c	hot and cold wall	
P	pressure, Pa	α	the direction of streaming step	
Pr	Prandtl number, $\nu/\chi$	$\overline{\alpha}$	the opposite direction of $\alpha$	
q	heat flux, W/m <sup>2</sup>		**	

The existing mathematical models for the phase change problem are mostly based on continuum approaches. The lattice Boltzmann method (LBM) is a relatively new approach that uses simple kinetic models to simulate complicated macroscopic transport phenomena. Owing to its mesoscopic nature, in comparison with conventional fluid dynamics solvers, it offers such advantages as simple calculation procedure, simple and efficient implementation for parallel computation, and easy and robust handling of complex geometries. LBM was first proposed by McNamara and Zanetti [19] in 1988. Chen and Doolen [20] conducted an overview of the lattice Boltzmann method for fluid flows. Then, the LBM was developed to solve a wide range of heat transfer problems [21]. Recently, phase change problems have also been investigated by the LBM [22]. Since LBM is inherently transient, it is an excellent approach for the investigation of transient phase change process. Specifically, the LBM solves the problems by evolution, which agrees well with the real physical melting process. In recent years, the application of LBM to phase change problems has been extensively investigated by many researchers [23–33].

It seems that Miller et al. [23] first developed a simple reaction model for the liquid—solid phase transition in the context of the lattice Boltzmann method with enhanced collisions. In his work, a two-dimensional test problem of Ga melting and a two-dimensional anisotropic growth of dendrites were presented. Jiaung et al. [24] proposed an extended lattice Boltzmann equation for the simulation of the phase-change problem governed by the heat conduction equation incorporated with enthalpy formation. Chakraborty and Chatterjee, in their outstanding works [16,22,25–28], applied the lattice Boltzmann technique to numerical simulation of conduction-dominated and convection-dominated phase change process (melting and solidification). Huber et al. [29] investigated the coupled thermal convection and pure-substance melting using a lattice Boltzmann method. The transition from conduction-dominated heat transfer to fully-

developed convection was analyzed. Gao et al. [30] performed a Lattice Boltzmann simulation of natural convection dominated melting in a rectangular cavity filled with porous media. Eshraghi et al. [31] developed an implicit lattice Boltzmann model for heat conduction with phase change, in which the latent heat source term was treated implicitly in the energy equation. Huang et al. [32] introduced an enthalpy based lattice Boltzmann method for phase change problems. In their works, the phase interface was traced by updating the total enthalpy, and the moving interface was treated by the immersed moving boundary scheme. Fuentes et al. [33] presented a new LBM-MRT hybrid model to simulate melting with natural convection in a phase change material. In the work, energy equation was solved by a finite difference method, whereas the fluid flow was solved by the multiple relaxation time (MRT) lattice Boltzmann method.

As mentioned above, phase change problems were numerically investigated by different models in a generalized lattice Boltzmann framework, but no detailed comparison between these models was provided in any reference work. Besides, most of lattice Boltzmann simulation for the phase change problems has been done in a simple cavity, while few studies have concerned more complex geometries. Therefore, the purpose of the present investigation is threefold: (i) to evaluate the capability of different lattice Boltzmann models for phase change process, i.e., the numerical stability of lattice Bhatnagar-Gross-Krook (LBGK) and multi-relaxation time (MRT) models for flow field, and the enthalpy-based lattice Boltzmann model with basic evolution variable of temperature (TLBM) and enthalpy (HLBM) for thermal field; (ii) to test the heat storage performance for three configurations consisting of a shell with different numbers (one, four and nine) of heat transfer tubes and different tubes arrangements (inline, staggered and a novel centrosymmetric design); (iii) to analyze the influence of the Rayleigh and Stefan numbers on the melting dynamics of shell and tube models with various arrangements.

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