International Journal of Heat and Mass Transfer 102 (2016) 637–644

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ijhmt

# A lattice Boltzmann model for heat transfer in heterogeneous media

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ARTICLE INFO

*Article history:*
Received 30 April 2016
Received in revised form 12 June 2016
Accepted 24 June 2016

*Keywords:*
Lattice Boltzmann method
Heat and mass transfer
Variable thermophysical properties
Heterogeneous media

ABSTRACT

So far the lattice Boltzmann (LB) method has matured as a powerful tool to address a diversity of heat and mass transfer challenges. For most practical applications, the variation of thermophysical properties of working media will influence the performance of industrial systems substantially. However, nowadays the efforts to improve the LB method to consider variable thermophysical properties of working media are quite sparse. In the present work we firstly analyze the shortcomings of the available LB approaches for modeling working fluid with variable thermophysical properties. Based on the analysis, a simple LB model is proposed to overcome these shortcomings. The feasibility and reliability of the new LB model have been validated by three simple but nontrivial benchmark tests. Although it is originally proposed to simulate fluid flow with variable thermophysical properties, the present model can be extended directly to some other research areas where variation of thermophysical properties of working media should be considered, such as conjugate heat transfer between solid materials.



## 1. Introduction

With the rapid development of computer science, numerical simulation has become a powerful, sometimes even a unique, tool to address a diversity of challenges in various practical applications. In the fields relevant to heat and mass transfer in fluid flow, computational fluid dynamics (CFD) techniques have been popularly adopted as a cost-effective way for system design, diagnosis and optimization. Due to the extreme complication of fluid flow in engineering, during the past decades various modeling approaches and numerical solvers have been continuously proposed to conquer the difficulties and to present a clearer physical picture of the investigated problems [1]. Among them, the lattice Boltzmann (LB) method has attracted significant attention owing to its some intrinsic advantages, such as modeling interaction, in a mesoscopic level, between different phases/components in multiphase/multicomponent flow and a thermodynamics-consistent description of turbulence [2]. Until now, LB-based approaches have been widely used not only to deepen our insight into numerous fundamental research areas [3–5], but also to constitute commercial software to optimize industrial processes [6]. On the topics relevant to heat transfer, the LB method has reached a great achievement over a wide range, such as enhanced heat transfer by nanofluid [7–10], micro-scale heat transfer [11–13] and conjugate heat transfer[14,15].

The LB method is a type of mesoscopic approach which implies it will not solve macroscopic governing equations directly as conventional CFD tools do, although macroscopic phenomena can be reproduced by it satisfactorily. All available LB-based approaches start from the so-called LB equation which can be regarded as a special discretization of the Boltzmann equation [2]. Through a multiscale expansion, some well-known macroscopic governing equations, such as the Euler and/or Navier–Stokes equation, can be recovered from the LB equation with different truncated errors [4]. Accordingly, in the recovered macroscopic governing equations all parameters representing the thermophysical properties of working media (e.g. specific heat capacity, thermal conductivity and dynamic viscosity) are determined through the multiscale expansion. In order to exactly match the macroscopic governing equations in CFD, a number of macroscopic quantities in the recovered macroscopic equations, including thermophysical properties of working media, are assumed to be constant or to vary slightly across the investigated domain. Originally, the LB method was developed as an alternative solver for isothermal low Mach number flow simulation, so such assumption was tenable. Later, the LB method was extended to model thermal flow and reaction flow [5]. Surprisingly, although the thermophysical properties of working media may be significantly different temporally and/or

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http://dx.doi.org/10.1016/j.ijheatmasstransfer.2016.06.082
0017-9310/

spatially in those scenarios, the above assumption has still been adopted implicitly. In spite of acceptable simulation results having been reproduced in some scenarios, it is not physical sound. Especially, in theory the applicable scope of these LB approaches has been limited not to exceed the relaxation of the above assumption too much, which can not meet the requirements of most practical applications.

Nowadays, the available open literature, attempting to model temporally/spatially different thermophysical properties of working media by the LB method, is quite sparse. Guo and Zhao [16] perhaps are the pioneers to consider how to model changeable dynamic viscosity of working fluid in the framework of the LB method. In Ref. [16], natural convection of a fluid with temperature-dependent viscosity was simulated. The influence of variable viscosity on heat transfer has been presented by the authors and it was observed the standard LB model's prediction, in which constant viscosity assumption adopted, would significantly deviate the real phenomena. However, there are still two implicit assumptions in Guo's LB model: (1) the density change of working fluid should be very small and (2) the specific heat capacity and thermal conductivity of working fluid should be constant. Unfortunately, in many industrial applications (e.g. combustion), these two assumptions can hardly be met. Recently, some scholars discussed how to model conjugate heat transfer by the LB method [17–22]. For conjugate heat transfer, the investigated domain is consisted of several different medium layers, and the specific heat capacity and/or thermal conductivity of the medium layers may be different with each other. However, their LB approaches can not treat spatially consecutive variation of thermophysical properties within any medium layer as in their models the thermophysical properties of each medium layer must to be spatially identical. On the other words, these LB models for conjugate heat transfer aim to handle interfaces between heterogeneous medium layers rather than to model variable thermophysical properties of working media.

This drawback has hampered the maturation of the LB method as an industrial-level CFD tool. In order to bridge this gap, in this work we try to establish a LB model which can deal with variable thermophysical properties of working media simply and efficiently. As shown by the above literature survey, this issue has been ignored by the LB community although it is extremely critical for practical applications. What should be emphasized is although in the present study we only take a single-relaxation-time LB model as an example to show how to address the variation of thermophysical properties of working media, the extension to its multiple-relaxation-time counterpart is straightforward [5,18].

## 2. LB model considering variation of thermophysical properties

The standard macroscopic governing equations for industrial fluid flow with variable thermophysical properties, in their tensor formulation, read [1]:

$$\partial_t \rho + \nabla_\alpha \rho u_\alpha = 0, \tag{1}$$

$$\partial_t \rho u_\alpha + \nabla_\beta \rho u_\alpha u_\beta = -\nabla_\alpha p + \nabla_\beta \mu(\nabla_\alpha u_\beta + \nabla_\beta u_\alpha), \tag{2}$$

$$\partial_t \rho C_p T + \nabla_\alpha \rho C_p T u_\alpha = \nabla_\alpha \lambda \nabla_\alpha T. \tag{3}$$

where $\rho, u_\alpha, p$ and $T$ are the density, velocity, pressure and temperature of working fluid. In addition, $\mu, \lambda$ and $C_p$ are the thermophysical properties of working fluid and they denotes the dynamic viscosity, thermal conductivity and constant pressure specific heat capacity, respectively.

However, the recovered macroscopic governing equations by the standard LB method read[2,4]:

$$\partial_t \rho + \nabla_\alpha \rho u_\alpha = 0, \tag{4}$$

$$\partial_t \rho u_\alpha + \nabla_\beta \rho u_\alpha u_\beta = -\nabla_\alpha p + \nabla_\beta \nu(\nabla_\alpha \rho u_\beta + \nabla_\beta \rho u_\alpha), \tag{5}$$

$$\partial_t \rho C_p T + \nabla_\alpha \rho C_p T u_\alpha = \nabla_\alpha \kappa \nabla_\alpha \rho C_p T. \tag{6}$$

where $\nu = \mu/\rho$ and $\kappa = \lambda/(\rho C_p)$ are the kinematic viscosity and thermal diffusivity of working fluid, respectively. One can observe there are obvious differences between the recovered macroscopic governing equations Eqs. (5) and (6) and the standard macroscopic governing equations Eqs. (2) and (3): firstly, the second term on the right side of Eq. (5) does not match that in Eq. (2) exactly; secondly, the last term of Eq. (6) is not the same as that in Eq. (3).

The second term on the right side of Eq. (5) $\nabla_\beta \nu(\nabla_\alpha \rho u_\beta + \nabla_\beta \rho u_\alpha)$ can be transformed as

$$\nabla_\beta \nu(\nabla_\alpha \rho u_\beta + \nabla_\beta \rho u_\alpha) = \nabla_\beta \mu(\nabla_\alpha u_\beta + \nabla_\beta u_\alpha) + \nabla_\beta \nu(u_\beta \nabla_\alpha \rho + u_\alpha \nabla_\beta \rho). \tag{7}$$

Therefore, Eq. (5) can approximate to Eq. (2) only when the spatial derivation of density is slight. For example, for isothermal low Mach number flow, there is $O(\nabla_\alpha \rho) \sim O(Ma^2)$ [23], so the equality Eq. (7) can be written as

$$\nabla_\beta \nu(\nabla_\alpha \rho u_\beta + \nabla_\beta \rho u_\alpha) = \nabla_\beta \mu(\nabla_\alpha u_\beta + \nabla_\beta u_\alpha) + O(Ma^2). \tag{8}$$

where $Ma$ is the Mach number. What should be emphasized is that the equality Eq. (8) may collapse in some low Mach number scenarios, such as in low Mach number combustion where the spatial derivation of density is large [24]. In the LB community, there is a commonly found mistake that many scholars take the low Mach number flow equivalent to $O(\nabla_\alpha \rho) \sim O(Ma^2)$. Strictly, such equivalence can stand only in isothermal low Mach number flow.

The last term in Eq. (6) can be rewritten as

$$\nabla_\alpha \kappa \nabla_\alpha \rho C_p T = \nabla_\alpha \lambda \nabla_\alpha T + \nabla_\alpha \kappa T \nabla_\alpha \rho C_p. \tag{9}$$

Accordingly, Eq. (6) can match Eq. (3) exactly only when $\nabla_\alpha \rho C_p = 0$ which implies at least $C_p$ should be a constant across the investigated domain. As discussed below, it is the reason why it is difficult to adopt the standard LB approach to treat conjugate heat transfer.

In order to recover the macroscopic governing equations Eqs. (1)–(3) exactly without the above restrictions, in the present study a double-distribution-function LB model is proposed. The present model is partially based on our previous LB model developed for low Mach number combustion simulation[24], in which the flow and scale (e.g. temperature) fields are solved by two sets of distribution functions, respectively.

### 2.1. Flow field

The evolving equation for the flow field reads

$$f_k(x_\alpha + ce_{\alpha k}\Delta t, t + \Delta t) - f_k(x_\alpha, t) = -\tau_u^{-1}\left[f_k(x_\alpha, t) - f_k^{(eq)}(x_\alpha, t)\right]. \tag{10}$$

where $f_k(x_\alpha, t)$ is the distribution function at space $x_\alpha$ and time $t$ with velocity $ce_{\alpha k}$ and $f_k^{(eq)}(\mathbf{x}, t)$ is the corresponding equilibrium distribution. $e_{\alpha k}$ is the discrete velocity direction, which depends on the lattice model adopted and $k = 0$ represents the stationary fluid particle. $\Delta x, \Delta t$ and $\tau_u$ are the lattice grid spacing, evolving time step and dimensionless relaxation time for the flow field, respectively. $c = \Delta x/\Delta t$ is the pseudo-fluid particle speed.

The equilibrium distribution in the present model is defined by

$$f_k^{(eq)} = \chi_k p + \rho s_k(u_\alpha), \tag{11}$$

where