Numerical Study of Cross Diffusion Effects on Double Diffusive Convection with Lattice Boltzmann Method

Xiaomei Yu¹, Zhaoli Guo¹, and Baochang Shi^{2,*}

¹ State Key Laboratory of Coal Combustion,
Huazhong University of Science and Technology,
Wuhan 430074 P.R. China
yuxiaomei_hust@126.com,
zlguo@mail.hust.edu.cn

² Department of Mathematics,
Huazhong University of Science and Technology,
Wuhan 430074 P.R. China
sbchust@126.com

Abstract. A lattice Boltzmann model is proposed to assess the impact of variable molecular transport effects on the heat and mass transfer in a horizontal shallow cavity due to natural convection. The formulation includes a generalized form of the Soret and Dufour mass and heat diffusion (cross diffusion) vectors derived from non-equilibrium thermodynamics and fluctuation theory. Both the individual cross diffusion effect and combined effects on transport phenomena are considered. Results from numerical simulations indicate that Soret mass flux and Dufour energy flux have appreciable effect and sometimes are significant. At the same time, the lattice Boltzmann model has been proved to be adequate to describe higher order effects on energy and mass transfer.

Keywords: lattice Boltzmann model; Soret effect; Dufour effect; Natural convection.

1 Introduction

Transport phenomena and thermo-physical property in fluid convection submitted to the influence of thermal and concentration horizontal gradients arise in many fields of science and engineering. The conservation equations which describe the transport of energy and mass in these fluid systems are well developed [1-3]. The energy flux includes contributions due to a temperature gradient (Fourier heat conduction), concentration gradient (Dufour diffusion) and a term which accounts for the energy transport as a result of each species having different enthalpies (species interdiffusion). The mass flux consists of terms due

* Corresponding author.

to a concentration gradient (Fickian diffusion), temperature gradient (Soret diffusion), Pressure gradient (pressure diffusion) and a term which accounts for external forces affecting each species by a different magnitude. However, most studies concerned on transport phenomena only considered the contributions due to Fourier heat conduction and Fickian diffusion.

The Soret mass flux and Dufour energy flux become significant when the thermal diffusion factor and the temperature and concentration gradients are large. Actually, Rosner [4] has stressed that Soret diffusion is significant in several important engineering applications. Similarly, Atimtay and Gill [5] have shown Soret and Dufour diffusion to be appreciable for convection on a rotating disc. An error as high as 30% for the wall mass flux is introduced when the Soret effect is not accounted for. Of particular interest, crystal growth from the vapor is sometimes carried out under conditions conducive to Soret and Dufour effects. As greater demands are made for tighter control of industrial processes, such as in microelectromechanical systems (MEMS) [6], second-order effects such as Soret and Dufour diffusion may have to be included.

In regard to actual energy and mass transport in double diffusive convection fluid systems which include Soret and Dufour cross diffusion effect, little, if any, complete and detailed work has been done. However, a few studies have considered the convection, within a vertical cavity, induced by Soret effects. The first study on this topic is due to Bergman and Srinivasan [7]. Their numerical results indicate that the Soret-induced buoyancy effects are more important when convection is relatively weak. The particular case of a square cavity under the influence of thermal and solutal buoyancy forces, which are opposing and of equal intensity, has been investigated by Traore and Mojtabi [8]. The Soret effect on the flow structures was investigated numerically. The same problem was considered by Krishnan [9] and Gobin and Bennacer [10] for the case of an infinite vertical fluid layer. The critical Rayleigh number for the onset of motion was determined by these authors. More recently, Ouriemi et al. [11] considered the case of a shallow layer of a binary fluid submitted to the influence of thermal and concentration horizontal gradients with Soret effects. Moreover, few studies have been concerned with the Soret and Dufour effects at the same time. Weaver and Viskanta numerically simulates these effects in a cavity [12]. Malashetty et al. [13] have performed a stability analysis of this problem. Because of the limited number of studies available, the knowledge concerning the influence of these effects on the heat and mass transfer and fluid flow is incomplete.

The lattice Boltzmann method (LBM) is a new method for simulating fluid flow and modeling physics in fluids. It has shown its power and advantages in wide range of situations for its mesoscopic nature and the distinctive computational features [14,15,16]. Contrary to the conventional numerical methods, the LBM has many special advantages in simulating physical problems. The objective of the present study is to develop an effective lattice Boltzmann model to examine the influences and the contributions of the Soret and Dufour effects on the natural convection with simultaneous heat and mass transfer across a horizontal shallow cavity. Based on the idea of the double distribution function

models for a fluid flow involving heat transfer, a generalized lattice Boltzmann model is proposed to solve the control equations with Soret and Dufour effects.

2 The Lattice Boltzmann Method for the Formulation of the Problem

The configuration considered in this study is a horizontal shallow cavity, of width H and length L . The top and bottom end walls were assumed to be adiabatic and impermeable to heat and mass transfer while the boundary conditions along the right and left side walls were subjected by Dirichlet conditions. Considering the Soret effects and Dufour effects, the dimensionless incompressible fluid equations for the conservation of mass, momentum, solutal concentration, and temperature, with the inclusion of the Boussinesq approximation for the density variation, are written as

$$\nabla \cdot \mathbf{u} = 0, \quad (1)$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla(\mathbf{u}) = -\nabla p + \left(\frac{Pr}{Ra}\right)^{1/2} \nabla^2 \mathbf{u} + Pr(T + \varphi C), \quad (2)$$

$$\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T = \frac{1}{\sqrt{Ra} Pr} (\nabla^2 T + D_{CT} \nabla^2 C), \quad (3)$$

$$\frac{\partial C}{\partial t} + \mathbf{u} \cdot \nabla C = \frac{1}{Le \sqrt{Ra} Pr} (\nabla^2 C + S_{TC} \nabla^2 T) \quad (4)$$

along with the boundary conditions where ρ and $\mathbf{u}$ are the fluid density and velocity, respectively. T is the temperature of the fluid.

The dimensionless variables are defined as

$$\mathbf{X} = \frac{\mathbf{X}}{H}, \quad t = \frac{t\sqrt{Ra}}{H^2/\alpha}, \quad \mathbf{u} = \frac{\mathbf{u}}{(\alpha/H)\sqrt{Ra}}, \quad p = \frac{p}{(\alpha^2/H^2)Ra}, \quad T = \frac{T - T_0}{\Delta T},$$

$$C = \frac{C - C_0}{\Delta C}, \quad Da = \frac{K}{H^2}, \quad Pr = \frac{\nu}{\alpha}, \quad Le = \frac{\alpha}{D}, \quad Ra = \frac{g\beta_T \Delta T H^3}{\nu \alpha}, \quad \varphi = \frac{\beta_C \Delta C}{\beta_T \Delta T}$$

Here, ν , α , D are the kinematic viscosity, thermal diffusivity and diffusion coefficient, respectively. The remaining notation is conventional. From the above equations it is observed that the present problem is governed by the thermal Rayleigh number Ra , buoyancy ratio φ , Lewis number Le , Prandtl number Pr , Dufour factor D_{CT} and Soret factor S_{TC} . In this paper, we concerned on the effect of Soret and Dufour factor. So other dimensionless variables will be kept at certain values.

Based on the idea of TLBGK model in [17], we take the temperature and concentration as passive scalar. Then the control equations of velocity, temperature and concentration can be treated individually. The evolution equation for the velocity field is similar to Ref. [18]

$$f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) - f_i(\mathbf{x}, t) = -\frac{1}{\tau} (f_i(\mathbf{x}, t) - f_i^{eq}(\mathbf{x}, t)) + \Delta t F_i(\mathbf{x}, t) \quad i = 0, \dots, b-1, \quad (5)$$

where $\mathbf{c}_i$ is the discrete particle velocity, F_i represents the force term, $f_i(\mathbf{x}, t)$ is the distribution function (DF) for the particle with velocity $\mathbf{c}_i$ at position $\mathbf{x}$ and time t , Δt is the time increment. τ is the nondimensional relaxation time and $f_i^{(eq)}$ is the equilibrium distribution function (EDF). The EDF must be defined appropriately such that the mass and momentum are conserved and some symmetry requirements are satisfied in order to describe the correct hydrodynamics of the fluid. In the $DnQb[19]$ models, the EDF is now defined as

$$f_i^{(eq)} = \alpha_i p + \omega_i \left[\frac{\mathbf{c}_i \cdot \mathbf{u}}{c_s^2} + \frac{\mathbf{u} \mathbf{u} : (\mathbf{c}_i \mathbf{c}_i - c_s^2 \mathbf{I})}{2c_s^4} \right]. \quad (6)$$

$$F_i = \frac{(\delta_{i2} + \delta_{i4})}{2c^2} \mathbf{c}_i Pr(T + \varphi C) \quad (7)$$

where ω_i is the weight and c_s is the sound speed. Both ω_i and c_s depend on the underlying lattice. Take the $D2Q9$ model for example, the discrete velocities are given by $\mathbf{c}_0 = 0$, and $\mathbf{c}_i = \lambda_i (\cos \theta_i, \sin \theta_i) c$ with $\lambda_i = 1$, $\theta_i = (i-1)\pi/2$ for $i = 1-4$, and $\lambda_i = \sqrt{2}$, $\theta_i = (i-5)\pi/2 + \pi/4$ for $i = 5-8$, and $c_s = c/\sqrt{3}$. $\omega_0 = 4/9$ and $\alpha_0 = -4\sigma/c^2$, $\omega_i = 1/9$ and $\alpha_i = \lambda/c^2$ for $(i = 1, 2, 3, 4)$, $\omega_i = 1/36$ and $\alpha_i = \gamma/c^2$ for $(i = 5, 6, 7, 8)$, respectively. Here, $\sigma = \frac{5}{12}$, $\lambda = \frac{1}{3}$, $\gamma = \frac{1}{12}$ is set [20] with best computation effects.

The fluid velocity $\mathbf{u}$ and pressure p are defined by the DF f_i

$$\mathbf{u} = \sum_i \mathbf{c}_i f_i = \sum_i \mathbf{c}_i f_i^{(eq)}, \quad p = \frac{c^2}{4\sigma} \left[\sum_{i \neq 0} f_i - \frac{2}{3} \frac{|\mathbf{u}|^2}{c^2} \right]. \quad (8)$$

Through the Chapman-Enskog expansion, the Eqs.(1),(2) can be obtained. The kinetic viscosity are given by $(\frac{Pr}{Ra})^{1/2} = \frac{(2\tau-1)}{6} c^2 \Delta t$.

Similarly, the LBGK equations for temperature and concentration fields with $D2Q5$ lattice are written as follows,

$$T_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) - T_i(\mathbf{x}, t) = -\frac{1}{\tau_T} [T_i(\mathbf{x}, t) - T_i^{(0)}(\mathbf{x}, t)] \quad (9)$$

$$S_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) - S_i(\mathbf{x}, t) = -\frac{1}{\tau_S} [S_i(\mathbf{x}, t) - S_i^{(0)}(\mathbf{x}, t)] \quad (10)$$

where T_i and S_i are the DF for the temperature field and concentration field, respectively. τ_T and τ_S are relaxation time corresponding to temperature DF and concentration DF trend to equilibrium. Just like the thoughts of constructing generalized LBGK model for Burgers equation [21], the EDF of temperature and concentration are defined as

$$\begin{aligned} T_i^{(0)} &= \frac{T}{4} [1 - d_0 + 2 \frac{\mathbf{c}_i \cdot \mathbf{u}}{c^2}] + \frac{D_{ST} S (1 - d_0)}{4}, \quad i \neq 0, \\ T_0^{(0)} &= T d_0 - D_{ST} S (1 - d_0), \quad i = 0. \end{aligned} \quad (11)$$

$$\begin{aligned} S_i^{(0)} &= \frac{S}{4} [(1 - l_0) \phi + 2 \frac{\mathbf{c}_i \cdot \mathbf{u}}{c^2}] + \frac{S_{TS} T (1 - l_0) \phi}{4}, \quad i \neq 0, \\ S_0^{(0)} &= S l_0 \phi - S_{TS} T (1 - l_0) \phi, \quad i = 0. \end{aligned} \quad (12)$$

The fluid temperature and concentration can be expressed by DFs,

$$T = \sum_i T_i = \sum_i T_i^{(eq)}, \quad S = \sum_i S_i = \sum_i S_i^{(eq)}. \quad (13)$$

It can be proved that the macroscopic temperature and concentration diffusion equations (3) and (4) can be recovered from LBE(9),(10). The corresponding thermal conduction coefficient, diffusion factor are

$$\frac{1}{\sqrt{RaPr}} = \frac{c^2}{2}(\tau_T - \frac{1}{2})\Delta t(1 - d_0), \quad (14)$$

$$\frac{1}{Le\sqrt{RaPr}} = \frac{c^2}{2}(\tau_T - \frac{1}{2})\Delta t(1 - d_0). \quad (15)$$

Here, d_0 and l_0 are adjustable parameters. Obviously, the lattice Boltzmann model can simulate the double diffusive not only including Fourier heat conduction and Fickian diffusion but also second-order cross diffusion by choosing adequate parameters.

3 Numerical Results and Discussion

Using the lattice Boltzmann model, we simulate the Soret and Dufour effects in double diffusive due to temperature and concentration gradient. Since the Soret and Dufour effects are diffusive processes, the Rayleigh number should not too high in order to decrease the advective flux relative to the diffusive flux. Furthermore, the buoyancy ratio is set to be $\varphi = 1$, which preserves the buoyancy forces induced by the thermal and solutal effects are of equal intensity. Simulation tests are conducted with varied Soret and Dufour factor and fixed Le and Pr number equal to 1 and 0.71, respectively. The lattice size is 128×256 with Ra equal to 10^3 .

Streamlines, isothermals and iso-concentration profiles varied with Dufour and Soret coefficients are shown in Fig. 1. The effect on mass, momentum and concentration transports made by varied cross diffusion coefficients can be observed obviously. The center velocity, local (averaged) Nusselt and Sherwood number on the left wall are showed in Fig. 2, Fig. 3 and Table 1 for detailed discussion, respectively. A positive (negative) value of Dufour and Soret coefficients decreases (increases) the value of the maximum velocity, and extends (reduces) the range of the velocity field. Moreover, Positive values for the Dufour and Soret coefficients yield solute concentrations below that of the free stream and so is the temperature, the opposite being also true. But when the Dufour coefficient is certain, the local Nusselt numbers decrease with Soret coefficients but local Sherwood number increase. While the Soret coefficient is certain, the local Nusselt numbers increase and the Sherwood number decrease instead. All curves show the expected behavior.

Fig. 1. Streamline, isotherms and iso-concentrations from left to right. From top to bottom, the Dufour and Soret coefficients are $(0, 0), (0, 0.5), (-0.5, -0.5), (-0.9, -0.9)$, respectively.

Fig. 2. The velocity components, u and v , along the vertical and horizontal lines through the center at different cross diffusion numbers (D_{CT}, S_{TC}) : a= $(0, -0.5)$; b= $(0, 0.0)$; c= $(0, 0.5)$; d= $(0, 0.9)$

Table 1. Averaged Nusselt and Sherwood number on the left wall varied with Soret and Dufour factors

(D, S)	(0,-0.5)	(0,0)	(0,0.5)	(0,0.9)	-0.5,0)	(0.5,0)	(0.9,0)	(-0.5,-0.5)	(0.5,0.5)	(0.9,0.9)
Nu	0.9570	0.7698	0.5608	0.3785	0.7465	0.7965	0.8200	1.0838	0.6532	0.6053
Sh	0.7465	0.7698	0.7965	0.8200	0.9570	0.5608	0.3785	1.0838	0.6532	0.6053

Fig. 3. Local Nusselt and Sherwood number on the left wall varied with cross diffusion numbers (The D_{CT} is equal 0 at the left two figures)

4 Summary

In this paper, a lattice Boltzmann model is proposed and used to assess the Soret and Dufour effects on the heat and mass transfer in a horizontal shallow cavity due to natural convection. The proposed model is constructed in the double distribution function framework. Cross diffusion effects are studied under the buoyancy counteracting flows and augmenting flows in shallow cavity with the lattice Boltzmann model. The numerical results show that Soret and Dufour effects have contributions to mass and energy flux. Sometimes, it may appear to be significant. Simulation results agree well with previous work. Moreover, it indicates that the lattice Boltzmann model is adequate to simulate molecular transport which even includes second-order effects. It seems that the lattice Boltzmann method is effective in describing higher order physical effects, which are important as the industry develops.

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