

Multicomponent lattice Boltzmann model from continuum kinetic theory

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We derive from the continuum kinetic theory a multicomponent lattice Boltzmann model with intermolecular interaction. The resulting model is found to be consistent with the model previously derived from a lattice-gas cellular automaton [X. Shan and H. Chen, *Phys. Rev. E* **47**, 1815 (1993)] but applies in a much broader domain. A number of important insights are gained from the kinetic theory perspective. First, it is shown that even in the isothermal case, the energy equipartition principle dictates the form of the equilibrium distribution function. Second, thermal diffusion is shown to exist and the corresponding diffusivities are given in terms of macroscopic parameters. Third, the ordinary diffusion is shown to satisfy the Maxwell-Stefan equation at the ideal-gas limit.

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Mass transport in a multicomponent fluid system is important in a wide range of practical applications. The classic hydrodynamic treatment of this problem is through Fick's equation or the Maxwell-Stefan equation coupled with the hydrodynamic equations [1]. When the number of components is nontrivial and none of the components can be assumed to be dilute, the solution of the hydrodynamic equations becomes challenging. More importantly, due to the recent rapid growth of microscale and nanoscale applications, understanding the mass transport at length scales comparable to the molecular mean free path becomes critical. In this flow regime, the continuum assumption breaks down and some kinetic descriptions have to be adopted.

After the intense development in the past two decades, the lattice Boltzmann (LB) method [2,3] has been established as a promising alternative for computational fluid dynamics. Various LB models for multiple components have been suggested since the early days [4,5]. In particular, a multicomponent model which incorporates intermolecular interactions was previously suggested [6] for modeling mixtures of arbitrary number of components. The central idea is that the distribution function of each component relaxes to a Maxwellian centered at a common velocity so chosen that, in the absence of long-range interactions, the total momentum of all components is conserved at each collision. This model satisfies the indistinguishable principle and the interaction model is Galilean invariant [7]. In addition, through the Chapman-Enskog analysis [8,9], it was shown that this model exhibits the diffusional behaviors such as the ordinary, the pressure, and the forced diffusions. Various diffusivities were also calculated according to Fick's model. However, due to its athermal lattice-gas origin, thermal diffusion cannot be considered, nor can any thermodynamic arguments.

When modeling mixtures of gases with different molecular weights, arguably the most important piece of physics underlying many interesting diffusional behaviors is the energy equipartition principle which implies in the present context that the averaged kinetic energy should be the same for particles of all components. As this principle is of a thermodynamic nature, it has not been explicitly implemented in

any of the existing multicomponent LB models which, as far as we are aware of, are all athermal. Nevertheless, out of the requirement that the equation of state (EoS) should be that of an ideal-gas mixture, it was suggested [9] that the equilibrium distribution function be so chosen to effectively make the averaged energy a constant for all components. The lack of a convincing justification for the equilibrium distribution function has led to the adoption of purely numerical and computationally more expensive approaches, such as the use of multiple lattices [10,11] and the introduction of additional tunable parameters [12]. It is also our suspicion that the absence of the energy equipartition has led to the reported deviation from Graham's law in the simulation of near-wall diffusion [13].

Inspired by the grad 13-moment theory [14], the LB method was reformulated as a special velocity-space discretization of the continuum Bhatnagar-Gross-Krook (BGK) equation by projecting it into a subspace of the velocity space spanned by the leading Hermite polynomials [15–18]. Taking advantage of the one-to-one mapping between the leading moments and the discrete distribution function values as established by the Gauss-Hermite quadrature, one can effectively solve for the leading moments from a discrete-velocity kinetic equation. Besides giving an alternative interpretation of the LB method, the formulation has recently led to both satisfactory clarifications of some long-standing issues and applications in flow regimes thought to be impossible for the LB method [19–22].

In this Rapid Communication, we derive the multicomponent LB model from the continuum kinetic theory with the assumption that the equilibrium distribution function of each component is a local Maxwellian with common velocity and temperature. The model obtained is not restricted to a particular lattice, contains no arbitrary constants, and naturally satisfies the principles of indifferentiability and energy equipartition. The mass transport is then analyzed and shown to recover the correct macroscopic behaviors. Finally, a number of concerns [23,24] about the validity of the mixing model are addressed in light of the insight gained in the present analysis. We would like to point out that, despite its long history in the classic kinetic theory, the development of multicomponent BGK models is still far from being satisfactory [25]. The model and analysis developed in the present work could also be applied in areas outside the LB method.

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Consider a mixture of S components of monatomic gases. The molecular weight of the σ th component is denoted by m_σ . Let \mathbf{x} and $\boldsymbol{\xi}$ be the position and velocity vectors, respectively, and t be the time. The single-particle distribution function of the σ th component, $f_\sigma(\mathbf{x}, \boldsymbol{\xi}, t)$, is defined such that $f_\sigma(\mathbf{x}, \boldsymbol{\xi}, t)d\mathbf{x}d\boldsymbol{\xi}$ is the probability of finding a particle of the σ th component in the element $d\mathbf{x}d\boldsymbol{\xi}$ of the phase space at time t . By definition, the number (mole) densities $n_\sigma(\mathbf{x}, t)$, mass densities $\rho_\sigma \equiv m_\sigma n_\sigma$, fluid velocity $\mathbf{u}(\mathbf{x}, t)$, and internal energy density per unit mass, $\epsilon(\mathbf{x}, t)$, are velocity moments of the distribution function,

$$\frac{\rho_\sigma}{m_\sigma} = n_\sigma = \int f_\sigma d\boldsymbol{\xi}, \quad \sigma = 1, \dots, S, \quad (1a)$$

$$\rho \mathbf{u} = \sum_{\sigma=1}^S m_\sigma \int f_\sigma \boldsymbol{\xi} d\boldsymbol{\xi}, \quad (1b)$$

$$\rho \epsilon = \frac{1}{2} \sum_{\sigma=1}^S m_\sigma \int f_\sigma |\boldsymbol{\xi} - \mathbf{u}|^2 d\boldsymbol{\xi}, \quad (1c)$$

where $\rho \equiv \sum_{\sigma=1}^S \rho_\sigma$ is the total mass density of the mixture and the barycentric flow velocity of the mixture, \mathbf{u} , is the measure of the mean momentum transfer.

It is convenient to consider higher velocity moments in a reference frame moving with velocity \mathbf{u} and introduce the *intrinsic velocity* $\mathbf{c} = \boldsymbol{\xi} - \mathbf{u}$. Of the most significance are the second moment \mathbf{P} and the contracted third moment \mathbf{Q} ,

$$P_{ij} \equiv \sum_{\sigma=1}^S m_\sigma \int f_\sigma c_i c_j d\mathbf{c}, \quad (2a)$$

$$Q_i \equiv \sum_{\sigma=1}^S m_\sigma \int f_\sigma c_i c^2 d\mathbf{c}, \quad (2b)$$

which are identified, respectively, with the stress tensor and the head flux due to molecular motion. The *internal* kinetic energy is the trace of the second moment,

$$\rho \epsilon = \frac{1}{2} \sum_{\sigma=1}^S m_\sigma \int f_\sigma c^2 d\mathbf{c} = \frac{1}{2} P_{ii}. \quad (3)$$

The per-component velocity \mathbf{u}_σ and the internal energy density ϵ_σ of the σ th component are defined as

$$n_\sigma \mathbf{u}_\sigma \equiv \int f_\sigma \boldsymbol{\xi} d\boldsymbol{\xi}, \quad n_\sigma \epsilon_\sigma \equiv \frac{1}{2} \int f_\sigma c^2 d\boldsymbol{\xi}. \quad (4)$$

For a mixture of ideal gases in D dimensions, the static pressure p can be taken as the averaged normal pressure,

$$p = P_{ij}/D = 2\rho\epsilon/D, \quad (5)$$

where the Einstein summation convention is used. In a mixture of monatomic gases, ϵ is related to the temperature T by the *energy equipartition principle*. Defining the total number density $n = \sum_{\sigma=1}^S n_\sigma$, we have

$$\rho \epsilon = (D/2)nk_B T, \quad (6)$$

where k_B is the Boltzmann constant. We therefore have the ideal-gas EoS,

$$p = nk_B T. \quad (7)$$

The evolution of the single-particle distribution functions is governed by the Boltzmann equations. Let \mathbf{g}_σ be the acceleration of the body force exerted on the particles of the σ th component. We have

$$\frac{\partial f_\sigma}{\partial t} + \boldsymbol{\xi} \cdot \nabla f_\sigma + \mathbf{g}_\sigma \cdot \nabla_{\boldsymbol{\xi}} f_\sigma = \Omega_\sigma, \quad \sigma = 1, \dots, S, \quad (8)$$

where Ω_σ on the right-hand side is the collision term representing the change in the distribution due to particle collisions. The collision term must conserve mass for each of the components, the total momentum, and the total kinetic energy,

$$\int \Omega_\sigma d\boldsymbol{\xi} = 0, \quad \sigma = 1, \dots, S, \quad (9a)$$

$$\sum_{\sigma=1}^S m_\sigma \int \Omega_\sigma \boldsymbol{\xi} d\boldsymbol{\xi} = \mathbf{0}, \quad (9b)$$

$$\sum_{\sigma=1}^S m_\sigma \int \Omega_\sigma \boldsymbol{\xi}^2 d\boldsymbol{\xi} = 0. \quad (9c)$$

The single-relaxation-time approximation [26] introduced by Bhatnagar *et al.* can also be extended to the multicomponent mixtures [27]. Here, we propose a simple relaxation model as

$$\Omega_\sigma = -(1/\tau_\sigma)[f_\sigma - f^{\sigma(eq)}], \quad \sigma = 1, \dots, S, \quad (10)$$

where τ_σ is the collision time of the σ th component and $f^{\sigma(eq)}$ is a local Maxwellian corresponding to the density n_σ , a common velocity \mathbf{u}' , and a common temperature T' ,

$$f^{\sigma(eq)} = n_\sigma \left(\frac{m_\sigma}{2\pi k_B T'} \right)^{D/2} \exp \left[-\frac{m_\sigma |\boldsymbol{\xi} - \mathbf{u}'|^2}{2k_B T'} \right]. \quad (11)$$

In the dimensionless units introduced in Ref. [18], all velocities are scaled by the velocity $c_0 = \sqrt{k_B T_0 / m_0}$, where T_0 and m_0 are, respectively, the reference temperature and the unit of molecular mass. If we define the dimensionless Maxwell-Boltzmann distribution as

$$f^{(MB)}(n, \mathbf{u}, \theta, \boldsymbol{\xi}) = \frac{n}{(2\pi\theta)^{D/2}} \exp \left[-\frac{|\boldsymbol{\xi} - \mathbf{u}|^2}{2\theta} \right], \quad (12)$$

the dimensionless $f^{\sigma(eq)}$ can be written as

$$f^{\sigma(eq)} = f^{(MB)}(n_\sigma, \mathbf{u}', \theta' / m_\sigma, \boldsymbol{\xi}), \quad (13)$$

where $\theta' = T' / T_0$, and all quantities are hereinafter to be understood as dimensionless.

Obviously the collision term given by Eqs. (10) and (13) satisfies Eq. (9a). To satisfy the rest of Eqs. (9), we substitute Eqs. (10) and (13) into Eqs. (9b) and (9c) to have

$$\sum_{\sigma=1}^S \frac{\rho_{\sigma}}{\tau_{\sigma}} (\mathbf{u}_{\sigma} - \mathbf{u}') = 0, \quad (14a)$$

$$\sum_{\sigma=1}^S \frac{\rho_{\sigma}}{\tau_{\sigma}} \left(2\epsilon_{\sigma} + u_{\sigma}^2 - \frac{D\theta'}{m_{\sigma}} - u'^2 \right) = 0, \quad (14b)$$

from which \mathbf{u}' and θ' can be solved as

$$\mathbf{u}' = \frac{\sum_{\sigma=1}^S \frac{\rho_{\sigma} \mathbf{u}_{\sigma}}{\tau_{\sigma}}}{\sum_{\sigma=1}^S \frac{\rho_{\sigma}}{\tau_{\sigma}}}, \quad (15a)$$

$$\theta' = \frac{\sum_{\sigma=1}^S \frac{\rho_{\sigma}}{\tau_{\sigma}} (2\epsilon_{\sigma} + u_{\sigma}^2 - u'^2)}{D \sum_{\sigma=1}^S \frac{n_{\sigma}}{\tau_{\sigma}}}. \quad (15b)$$

As far as we know, Eq. (15a) was first suggested in Ref. [8] and Eq. (15b) was a natural extension. As pointed out by an anonymous referee, the same expressions can also be obtained as a special case from a more general BGK model [25], and the discussions therein on the H theorem and hydrodynamics apply here as well.

Equations (8), (10), (12), (13), and (15) define our BGK model for multiple components. A few important observations can be made immediately. First, when all components are identical, i.e., $\tau_{\sigma} = \tau$ and $m_{\sigma} = m$, the system reduces to the single-component BGK equation and satisfies the indistinguishability principle. Second, \mathbf{u}' and θ' generally do not equal \mathbf{u} and θ unless either the velocities or temperatures of all components are the same, or all the relaxation times are the same. As the mixture approaches equilibrium, all \mathbf{u}_{σ} and θ_{σ} relax to \mathbf{u}' and θ' , which ensures that \mathbf{u}' and θ' eventually approach \mathbf{u} and θ . Third, the m_{σ} factor in Eq. (13) is the direct consequence of the energy equipartition principle. It dictates that heavier particles have smaller averaged thermal speed, so that the averaged kinetic energy, and thus the temperature, is the same for particles of all components.

The multicomponent lattice BGK (LBGK) model on a discretized space-time can now be derived following the same derivation for single-component [18]. The continuum model is first discretized in velocity space by projecting Eq. (8) into the Hilbert space spanned by the leading Hermite polynomial. Choosing the set of discrete velocities $\{\xi_a : a = 1, \dots, d\}$, and the corresponding weights $\{w_a : a = 1, \dots, d\}$, so that together they form a Gauss-Hermite quadrature which ensures that relevant moments can be exactly evaluated using f_a^{σ} , the dynamics of the leading moments can then be recovered from that of the discrete distribution function obtained by evaluating Eq. (8). After defining $f_a^{\sigma} = w_a f_{\sigma}(\xi_a) / \omega(\xi_a)$ and approximating the left-hand side of Eq. (8) by a finite-difference operator, the multicomponent LBGK equations are

$$f_a^{\sigma}(\mathbf{x} + \xi_a, t + 1) - f_a^{\sigma}(\mathbf{x}, t) = - (1/\tau_{\sigma}) [f_a^{\sigma} - f_a^{\sigma(eq)}] + F_a^{\sigma}, \quad (16)$$

$$\sigma = 1, \dots, S, \quad a = 1, \dots, d,$$

where F_a^{σ} are the body-force contribution [18] written here as a part of the collision term, and $f_a^{\sigma(eq)} = \tilde{f}(n_{\sigma}, \mathbf{u}', \theta' / m_{\sigma})$, where \tilde{f} is a finite-order truncated Hermite expansion of the Maxwellian, given originally as Eqs. (18) and (19) in Ref.

[17], and later in more elaborated forms as Eq. (3.23) in Ref. [18] and Eq. (14) in Ref. [20]. Note that in contrast with the conventional Taylor expansion in small velocity, the temperature appears as a dynamic variable on par with the velocity, allowing thermal effects to be incorporated into the LBGK dynamics consistently [19,28].

As a special case, if the energy equation is of no interest and the Mach number is sufficiently small, it is sufficient to use the following second-order Hermite expansion of Eq. (12):

$$f_a^{\sigma(eq)} = w_a n_{\sigma} [1 + u_a + [u_a^2 - u'^2 + \gamma_{\sigma}(\xi_a^2 - D)]/2], \quad (17)$$

where $u_a = \mathbf{u}' \cdot \xi_a$, and $\gamma_{\sigma} = \theta' / m_{\sigma} - 1$, with \mathbf{u}' given by Eqs. (15) and θ' simply set at a constant value. This special case recovers the multicomponent model in Refs. [6,8,9]. Noticing that the numerical constant d_0 in the previous model was identified with the quantity $1 - 2\theta$ [18], the requirement of $1 - d_{\sigma} \sim 1/m_{\sigma}$ to recover the idea-gas EoS in Ref. [9] is simply $\theta_{\sigma} \sim 1/m_{\sigma}$ as required by the equipartition principle. We also note that essentially the same approach is used in Ref. [10] as the same-lattice-speed scheme and in Refs. [12,29,30]. Comparing with the other approach of handling particles with different molecular weights by using different lattices [10,11], the model of adjusting the temperature in equilibrium distribution [9] is not only simpler, more versatile, and computationally efficient in handling large number of components, but more importantly also consistent with the continuum kinetic theory and reflects the essence of the underlying physics.

We now proceed to the calculation of mass transport coefficients. We first note that the discussion of energy equipartition so far is within the limit of ideal gases since, despite many attempts, all existing non-ideal-gas LB models do not have exact microscopic energy conservation. Whether or not a Hamiltonian with potential contribution can be written down is at this time still unknown. However, the transport coefficients in a fluid with nonlocal interaction can be readily calculated. In Ref. [6], the non-ideal-gas effect can be modeled by an interaction force between particles on neighboring sites. The force of such a nature on the σ th component at \mathbf{x} is

$$\mathbf{F}_{\sigma} = - \psi_{\sigma}(\mathbf{x}) \sum_{s=1}^S G_{\sigma s} \sum_{a=1}^d \psi_s(\mathbf{x} + \mathbf{e}_a) \mathbf{e}_a, \quad (18)$$

where $\psi_{\sigma} = \psi_{\sigma}(n_{\sigma})$ are the component-specific *pseudopotentials*, $G_{\sigma s}$ is a Green's function which regulates the differences among interactions between different pairs of components, and \mathbf{e}_a are the vectors pointing from a lattice site to the interacting neighbors. With the interaction, the EoS of the mixture becomes

$$p = n\theta + \frac{1}{2} \sum_{\sigma=1}^S \sum_{s=1}^S G_{\sigma s} \psi_{\sigma}(n_{\sigma}) \psi_s(n_s), \quad (19)$$

where the second term is the potential contribution. Using the multiple-component Chapman-Enskog calculation [8], we obtain the mass flux of the σ th component as

$$\mathbf{j}_{\sigma} \equiv \rho_{\sigma}(\mathbf{u}_{\sigma} - \mathbf{u}) = \tau_{\sigma} \mathbf{G}_{\sigma} - (\tau_{\sigma} - 1/2) \Pi_{\sigma} - x_{\sigma} \sum_{s=1}^S \left[\left(\tau_s + \frac{1}{2} \right) \mathbf{G}_s - \tau_s \Pi_s \right], \quad (20)$$

where $x_\sigma \equiv \rho_\sigma/\rho$ is the *mass fraction*, $\mathbf{G}_\sigma = \mathbf{F}_\sigma + \rho_\sigma \mathbf{g}_\sigma$ is the total force, and

$$\Pi_\sigma = x_\sigma \left(-\nabla p + \sum_{s=1}^S \mathbf{G}_s \right) + \nabla(n_\sigma \theta). \quad (21)$$

First, by letting $\nabla p = \nabla n_\sigma = \mathbf{G}_\sigma = 0$ in Eq. (20), we have

$$\mathbf{j}_\sigma = -n \left[\left(\tau_\sigma - \frac{1}{2} \right) c_\sigma - x_\sigma \sum_{s=1}^S \tau_s c_\sigma \right] \nabla \theta, \quad (22)$$

where $c_\sigma \equiv n_\sigma/n$ is the *mole fraction* of the σ th component. When the relaxations are not all the same, a mass flux will be induced by a temperature gradient.

We now show that the Maxwell-Stefan law is satisfied in an ideal-gas mixture. With body force, pressure, and temperature gradients all vanishing, Eq. (20) reduces to

$$\rho_\sigma (\mathbf{u}_\sigma - \mathbf{u}) = - \left(\tau_\sigma - \frac{1}{2} \right) \theta \nabla n_\sigma + x_\sigma \theta \sum_{s=1}^S \tau_s \nabla n_s. \quad (23)$$

Dividing both sides by ρ_σ and taking the difference between components α and β , after defining $\phi_\sigma = (\tau_\sigma - 1/2)/m_\sigma$,

$$\mathbf{u}_\alpha - \mathbf{u}_\beta = \theta [\phi_\beta \nabla n_\beta / n_\beta - \phi_\alpha \nabla n_\alpha / n_\alpha]. \quad (24)$$

Noticing that $\sum_{\beta=1}^S \nabla c_\beta = 0$, and the constraint of homogeneous pressure and temperature implies $\nabla n = 0$ for ideal-gas mixtures, on multiplying both sides by $c_\alpha c_\beta / \theta \phi_\beta$ and summing over β , the equation above reduces exactly to the Maxwell-Stefan equation,

$$\sum_{\beta=1}^S \frac{c_\alpha c_\beta (\mathbf{u}_\alpha - \mathbf{u}_\beta)}{\mathcal{D}_{\alpha\beta}} = -\nabla c_\alpha, \quad (25)$$

where the mutual diffusivity $\mathcal{D}_{\alpha\beta}$ is given by

$$\mathcal{D}_{\alpha\beta} = \theta \phi_\alpha \phi_\beta \sum_{\sigma=1}^S \frac{c_\sigma}{\phi_\sigma}. \quad (26)$$

Finally, since the publications of Refs. [6,8,9] a number of concerns have arisen [23,24] over (i) the validity of modeling multicomponent collision process using a single collision term, which results in coupled transport coefficients; (ii) the dependency of \mathbf{u}' on the relaxation times; (iii) variations of transport coefficients modeled via nonlocal interaction; and (iv) the inability for each component to have its own viscosity if $\mathbf{u}' = \mathbf{u}$ is required. To address these concerns we give the following remarks. As shown earlier, the macroscopic variables \mathbf{u}' and θ' only represent an intermediate target of the relaxation process. As the system approaches the final equilibrium, they approach the barycentric velocity and temperature. There is a little justification to ensure $\mathbf{u}' = \mathbf{u}$ and $\theta' = \theta$ during the whole relaxation process. Without the constraint of $\mathbf{u}' = \mathbf{u}$, each component can have its own relaxation time and transport coefficients while the conservation laws are satisfied. For the same reason, it is neither necessary for \mathbf{u}' and θ' to be solely determined by macroscopic parameters. Instead, as intermediate quantities, it is not surprising that they depend on the relaxation times. Of course, the detailed forms of the transport coefficients, particularly the ratios among them, can deviate from the corresponding predictions of the full Boltzmann equation. Nevertheless, the top priority here is to construct a model that recovers the correct macroscopic behaviors, i.e., the principles of indiffereability and energy equipartition and the correct hydrodynamic equations. In addition, it is well known that for a low-density ideal gas the transport coefficients are coupled together and the Prandtl and Schmidt numbers vary only in a narrow range. The wide variations and complicated dependencies on other macroscopic parameters of the transport coefficients observed in liquids and other complex fluids are essentially due to the effects of long-range interactions and finite exclusion volumes. The most natural way to model such complexities is perhaps via the modeling of the same microscopic physics, and such a capability is highly desirable.

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