Lattice Boltzmann model for thermal binary-mixture gas flows

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A lattice Boltzmann model for thermal gas mixtures is derived. The kinetic model is designed in a way that combines properties of two previous literature models, namely, (a) a single-component thermal model and (b) a multicomponent isothermal model. A comprehensive platform for the study of various practical systems involving multicomponent mixture flows with large temperature differences is constructed. The governing thermohydrodynamic equations include the mass, momentum, energy conservation equations, and the multicomponent diffusion equation. The present model is able to simulate mixtures with adjustable Prandtl and Schmidt numbers. Validation in several flow configurations with temperature and species concentration ratios up to nine is presented.

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I. INTRODUCTION

The study of advanced energy conversion systems requires the use of physical models capable of describing several complex processes. The lattice Boltzmann (LB) method has become a very popular platform for the simulation of fluid flows in a variety of applications that range from laminar and turbulent flows in simple and complex geometries to multiphase and particle flows [1–4].

For the study of multicomponent flows, there has been a continuous effort in recent years to derive more accurate and more stable models, leading to many different approaches [5–18]. The fundamental difference when compared to the single-component formulation is the use of two or multiple relaxation parameter collision models, for example, to control separately the viscous dynamics and the molecular diffusion of the components. So far, success has been mainly in the nonthermal multicomponent LB modeling. The difficulty in obtaining numerically stable thermal models on the standard $D2Q9$ and $D3Q27$ lattices hindered further extension of multicomponent models and excluded the energy balance description on these simple lattices. In Ref. [16], some basic theoretical aspects concerning the derivation of a thermal multicomponent LB model, which can be applied only to extended lattice velocity sets, were presented. A special case of that model, where the energy equation is of no interest and the Mach number is sufficiently small, was detailed therein.

Recently, a single-component thermal LB model was proposed [19]. For two-dimensional flows, the $D2Q9$ lattice has been used, while for three-dimensional flows, a $D3Q27$ equivalent lattice has been developed. By construction, this formulation exhibits Galilean invariance, reference temperature independence, and rotational isotropy, which are some features that are unique regarding models constructed on these lattices. Moreover, the correct description of thermohydrodynamics allows the simulation of flows with large temperature and density variations. This model was also used in Ref. [20] for the simulation of combustion. In that case,

it was coupled with a LB scheme that solved the advection-diffusion equation of species and considered compressibility effects.

A multicomponent isothermal LB model with some remarkable features was proposed in Refs. [12,13]. Among others, this model can describe microflows, is able to simulate components with large mass ratios, and satisfies the indifferenciability principle.

Constructing a model that combines the advantages of the aforementioned models allows for a better description of the underlying processes in many mixture flows, wherein temperature gradients cannot be neglected. These types of processes include, among others, small energy converters (e.g., fuel cells) and microcombustors for portable power generation. In this paper, a thermal binary-mixture LB model on the $D2Q9$ lattice is constructed and studied in detail. The governing thermohydrodynamic equations include the mass, momentum, energy conservation equations, and the binary-mixture diffusion equation. Prandtl and Schmidt numbers are adjustable and simulation results suggest that this model is a suitable candidate for the simulation of heat transfer and reacting flows.

The paper is organized as follows. In Sec. II, the theoretical derivation of the model is presented. In Sec. III, the macroscopic limit of the model is calculated via a Chapman-Enskog analysis, and the deviation from the continuum thermal-mixture and Navier-Stokes equations is outlined with the help of Appendix A. In Secs. IV and V, a way to improve the accuracy of the model by introducing specifically designed terms at the level of the lattice BGK equation is proposed. Also, an approach to control the Prandtl number is outlined. In Secs. VI and VII, validation and benchmarking of the proposed model against analytic solutions and other numerical tools is presented.

II. THERMAL BINARY-MIXTURE MODEL

The derivation of the new thermal-mixture model is in line with Refs. [12,19]. A binary gas mixture, which is composed of two species A and B , is under consideration. Each species of the gas mixture is represented by one particle distribution function f_j , with $j = A, B$. Each species obeys its own

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BGK-type kinetic equation, which can be expressed as

$$\partial_t f_{ji} + c_{ji\alpha} \partial_\alpha f_{ji} = -\frac{1}{\tau_1} (f_{ji} - f_{ji}^*) - \frac{1}{\tau_2} (f_{ji}^* - f_{ji}^{eq}), \quad (1)$$

where $i = 0, \dots, N$ is the number of discrete velocities $c_{ji\alpha}$, and $\alpha = \{x, y, z\}$. The current study is based on the standard $D2Q9$ lattice, where $N = 9$ and $\alpha = \{x, y\}$. Therefore, the set of discrete velocities can be written as

$$\begin{aligned} c_{jix} &= c_j \{0, 1, 0, -1, 0, 1, -1, -1, 1\}, \\ c_{jiy} &= c_j \{0, 0, 1, 0, -1, 1, 1, -1, -1\}, \end{aligned} \quad (2)$$

with $c_j = \sqrt{1/M_j}$, and M_j is the molar mass of component j . The heavier species has slower characteristic velocity compared to the lighter one. This, in turn, imposes in the discretization process two different lattices, one for each species (for the numerical implementation, see Appendix B). The BGK relaxation process is split in two parts following the quasiequilibrium (QE) concept, similar to Refs. [21–23]. The first part is characterized by a relaxation toward an intermediate state, represented by f_{ji}^* , while the second part describes a relaxation toward the thermodynamic equilibrium, represented by f_{ji}^{eq} . The relaxation processes are governed by the characteristic times τ_1 and τ_2 , which are related to the macroscopic transport coefficients of the model.

The relevant moments of each species, which are useful in the analysis that follows, are the density, momentum, energy, pressure tensor, third order moment, third order contracted moment, and fourth order contracted moments,

$$\begin{aligned} \rho_j &= \sum_{i=0}^8 f_{ji}, \quad J_{j\alpha} = \sum_{i=0}^8 f_{ji} c_{ji\alpha}, \quad E_j = \sum_{i=0}^8 f_{ji} c_{ji}^2, \\ P_{j\alpha\beta} &= \sum_{i=0}^8 f_{ji} c_{ji\alpha} c_{ji\beta}, \quad Q_{j\alpha\beta\gamma} = \sum_{i=0}^8 f_{ji} c_{ji\alpha} c_{ji\beta} c_{ji\gamma}, \\ q_{j\alpha} &= \sum_{i=0}^8 f_{ji} c_{ji\alpha} c_{ji}^2, \quad R_{j\alpha\beta} = \sum_{i=0}^8 f_{ji} c_{ji\alpha} c_{ji\beta} c_{ji}^2. \end{aligned} \quad (3)$$

The equilibrium distribution function f_{ji}^{eq} is calculated as a minimizer of the H function [12,19,24,25],

$$H = \sum_j \sum_{i=0}^8 f_{ji} \ln f_{ji},$$

under specific constraints. The constraints applied in this case are the species density ρ_j , the momentum of the mixture J_α , and the energy of the mixture E :

$$\begin{aligned} \sum_{i=0}^8 f_{ji}^{eq} &= \rho_j, \quad \sum_j \sum_{i=0}^8 f_{ji}^{eq} c_{ji\alpha} = J_\alpha^{eq} = J_{A\alpha} + J_{B\alpha}, \\ \sum_j \sum_{i=0}^8 f_{ji}^{eq} c_{ji}^2 &= \sum_j \sum_{i=0}^8 f_{ji} c_{ji}^2 = 2CT + \frac{J^2}{\rho} = E_A + E_B, \end{aligned} \quad (4)$$

where T is the temperature of the mixture and C is the total concentration of the mixture defined as $C = \sum_j^{A,B} C_j = \sum_j^{A,B} \rho_j / M_j$. An additional constraint (guiding constraint) is

introduced in order to increase the accuracy of the higher order moments, similar to the derivation of the guided-equilibrium populations of the single-component thermal model [19,26–28]:

$$\begin{aligned} P_{\alpha\beta}^{eq} &= \sum_j \sum_{i=0}^8 f_{ji}^{eq} c_{ji\alpha} c_{ji\beta} = CT\delta_{\alpha\beta} + \frac{J_\alpha J_\beta}{\rho}, \\ P_{A\alpha\beta}^{eq} &= C_A T \delta_{\alpha\beta} + \rho_A \frac{J_\alpha J_\beta}{\rho^2}, \quad P_{B\alpha\beta}^{eq} = C_B T \delta_{\alpha\beta} + \rho_B \frac{J_\alpha J_\beta}{\rho^2}. \end{aligned}$$

The result of the minimization process produces the following form for the equilibrium populations of each species:

$$\begin{aligned} f_{ji}^{eq}(\rho_j, u, T) &= \rho_j \prod_{\alpha=x,y} \frac{(1 - 2c_{0i\alpha}^2)}{(2)^{c_{0i\alpha}^2}} [(c_{0i\alpha}^2 - 1) \\ &\quad + \sqrt{M_j} c_{0i\alpha} u_\alpha + M_j u_\alpha^2 + T], \end{aligned} \quad (5)$$

where c_{0i} is defined via Eq. (2) by setting $c_j = 1$. The velocity of the mixture is defined as u_α and is related to the momentum of the mixture via $u_\alpha = J_\alpha / \rho$. The moments of the equilibrium distribution function are in agreement with the ones predicted by the kinetic theory of gases [Maxwell Boltzmann form (MB)] up to the second order. Deviation appears in the higher order moments and is marked as $Q'_{\alpha\beta\gamma}$, q'_α , and $R'_{\alpha\beta}$ (see Appendix A). The origin of this deviation is the simplicity of the lattice itself; however, its effect at the macroscopic limit can be neutralized by the proper introduction of counterterms at the level of the lattice BGK equation, similar to the thermal single-component model.

The auxiliary state f^* is derived by minimizing the H functional under different constraints. The constraint of total momentum conservation is replaced by the individual species momentum conservation,

$$J_{j\alpha}^* = \sum_{i=0}^8 f_{ji}^* c_{ji\alpha} = \sum_{i=0}^8 f_{ji} c_{ji\alpha} = J_{j\alpha}, \quad (6)$$

and the result of the minimization is quite similar to the equilibrium distribution function and reads as

$$\begin{aligned} f_{ji}^*(\rho_j, u_j, T) &= \rho_j \prod_{\alpha=x,y} \frac{(1 - 2c_{0i\alpha}^2)}{(2)^{c_{0i\alpha}^2}} [(c_{0i\alpha}^2 - 1) \\ &\quad + \sqrt{M_j} c_{0i\alpha} u_{j\alpha} + M_j u_{j\alpha}^2 + T], \end{aligned} \quad (7)$$

where $u_{j\alpha}$ is the velocity of species j defined as $u_{j\alpha} = J_{j\alpha} / \rho$. Using the aforementioned distribution functions, it is possible to study the macroscopic thermohydrodynamic limit. This is the subject of the next section. Extension from a binary thermal-mixture model to a multispecies thermal model is straightforward.

III. MACROSCOPIC LIMIT

In this section, the macroscopic limit of the model is presented. The moments of the kinetic Eq. (1) are combined with the moments of the equilibrium populations of Eqs. (5) and (7) to provide the basic equations that describe the model behavior. The total density, momentum, and energy of the mixture are the conserved quantities, as depicted in the

following equations:

$$\partial_t \rho + \partial_\alpha J_\alpha = 0, \quad \partial_t J_\alpha + \partial_\beta P_{\alpha\beta} = 0, \quad \partial_t E + \partial_\alpha q_\alpha = 0. \quad (8)$$

The species momentum equation reads

$$\partial_t J_{j\alpha} + \partial_\beta P_{j\alpha\beta} = -\frac{1}{\tau_2} \left(J_{j\alpha} - \frac{\rho_j}{\rho} J_\alpha \right), \quad (9)$$

where the right-hand side describes the diffusion flux $V_{j\alpha} = J_{j\alpha} - (\rho_j/\rho)J_\alpha$. A property of the diffusion process in mixtures is that locally the total mixture diffusion flux is equal to zero: $\sum_j V_{j\alpha} = 0$. For the binary mixture under consideration, this implies $V_{A\alpha} = -V_{B\alpha}$.

The macroscopic limit of the model is identified via the Chapman-Enskog asymptotic analysis (for details, see Appendix A). The result for the momentum equation reads

$$\begin{aligned} \partial_t J_\alpha + \partial_\alpha P + \partial_\beta \left[\frac{J_\alpha J_\beta}{\rho} - \mu \partial_\gamma \left(\frac{J_\alpha}{\rho} \delta_{\beta\gamma} + \frac{J_\beta}{\rho} \delta_{\alpha\gamma} - \frac{J_\gamma}{\rho} \delta_{\alpha\beta} \right) \right] \\ + \partial_\beta P''_{\alpha\beta} = 0. \end{aligned} \quad (10)$$

In this expression, the pressure is defined as $P = CT$, and the dynamic viscosity is

$$\mu = \tau_1 CT. \quad (11)$$

Term $P''_{\alpha\beta}$ represents the deviation of the current model's momentum equation compared to the Navier-Stokes momentum equation. This deviation is a direct consequence of the simplicity (symmetry) of the $D2Q9$ lattice. Such deviation is inherent in all $D2Q9$ lattice schemes. Its manifestation invalidates the Galilean invariance by giving rise to the so-called “cubic” error in velocity $O(u^3)$, as has been already outlined by many authors [4,27,29–33]. The equilibrium populations cannot be further improved in a way that could remove this deviation. Hence, a correction scheme is added at the level of the BGK equation, similar to that in Ref. [19], and this will be the subject of the next section.

The model recovers the Maxwell-Stefan diffusion equation as

$$\partial_\alpha X_A = \frac{X_A X_B}{D_{AB}} \left(\frac{J_{B\alpha}}{\rho_B} - \frac{J_{A\alpha}}{\rho_A} \right) + (Y_A - X_A) \frac{\partial_\alpha P}{P}, \quad (12)$$

where X_j is the mole fraction of species j , $X_j = C_j/C$, and Y_j is the mass fraction $Y_j = \rho_j/\rho$. The mass diffusivity D_{AB} is equal to

$$D_{AB} = \frac{\tau_2 X_A X_B P}{m_{AB}},$$

with $m_{AB} = \rho_A \rho_B / \rho$ being the reduced mass. The Schmidt number of the mixture is a controllable parameter and for the present model is defined as

$$\text{Sc} = \frac{\mu}{D_{AB} \rho} = \frac{Y_A Y_B}{X_A X_B} \frac{\tau_1}{\tau_2}. \quad (13)$$

It is worth mentioning that according to the quasiequilibrium concept, the inequality $\tau_1 < \tau_2$ is required in order to prove the existence of the H theorem, as explained in Refs. [21,22]. This inequality suggests that for the simulation of the whole range of Schmidt numbers, a second collision

model needs to be constructed, as done in Refs. [13,34]. In this paper, we choose to work in a large range of Schmidt numbers, solely with the model presented in this section (either when $\tau_1 < \tau_2$ or $\tau_1 > \tau_2$). Moreover, we have not observed so far any kind of numerical instabilities that could be attributed to this inequality.

The equation describing the temperature evolution is identified as

$$\begin{aligned} \partial_t T = -u_\alpha \partial_\alpha T - T \partial_\alpha u_\alpha + \frac{1}{C} \partial_\alpha (k \partial_\alpha T) - \frac{1}{C} \nabla \\ \cdot \left(\sum_j^{A,B} 2TC_j \mathbf{U}_j \right) + \frac{\mu}{C} \partial_\alpha u_\beta (\partial_\alpha u_\beta + \partial_\beta u_\alpha - \partial_\gamma u_\gamma \delta_{\beta\alpha}) \\ - \frac{1}{2C} \partial_\alpha (q'_\alpha + q''_\alpha). \end{aligned} \quad (14)$$

In this expression, $\mathbf{U}_j = \mathbf{V}_j/\rho_j$ is the diffusion velocity. The thermal conductivity κ of the model is identified as

$$\kappa = 2\tau_1 CT \sum_j^{A,B} \frac{X_j}{M_j}. \quad (15)$$

Terms q'_α and q''_α represent the deviation of the current bare model from the continuum energy equation (Appendix A). The fourth term in the right-hand side of Eq. (14) is the enthalpy flux relative to the average motion of the mixture. It accounts for energy changes due to composition changes, which occur during species diffusion. Its importance was highlighted in Ref. [35], where it was shown that it prevented local violations of the entropy condition. More specifically, in combustion applications, omission of this term can generate spurious temperature gradients and violation of the energy conservation.

Knowing the exact analytic form of the deviations of Eqs. (10) and (14) allows one to design and apply a correction scheme that recovers the desired macroscopic limit.

IV. CORRECTION SCHEME

The thermohydrodynamic macroscopic limit of the bare model exhibits a certain deviation when compared to the Navier-Stokes and energy equations. This deviation is a consequence of the $D2Q9$ lattice symmetry, and the lack of sufficient degrees of freedom (discrete velocities), which are needed to correctly reproduce the higher order equilibrium moments. For small concentration, velocity, and temperature gradients, the deviation attains its minimum. For realistic flows with large gradients, this deviation is appreciable. In this section, a correction procedure that guarantees correct macroscopic limit, similar to the one used for the single-component thermal model [19], is presented in detail.

The BGK-type equation (1) is modified and is now equipped with specifically designed counterterms, whose purpose is to remove this deviation,

$$\begin{aligned} \partial_t f_{ji} + c_{ji\alpha} \partial_\alpha f_{ji} = -\frac{1}{\tau_1} (f_{ji} - f_{ji}^*) - \frac{1}{\tau_2} (f_{ji}^* - f_{ji}^{eq}) \\ + \psi_{ji} + \phi_{ji}. \end{aligned} \quad (16)$$

The terms ψ_{ji} are responsible for the momentum equation, while the terms ϕ_{ji} deliver an exact energy equation and allow

control of the Prandtl number. These terms are defined using the vectors Ψ_{jx} , Ψ_{jy} , and Φ_j :

$$\begin{aligned}\Psi_{jx} &= \frac{1}{4c_j} [0, 4, 0, -4, 0, -1, 1, 1, -1], \\ \Psi_{jy} &= \frac{1}{4c_j} [0, 0, 4, 0, -4, -1, -1, 1, 1], \\ \Phi_j &= \frac{1}{8c_j^2} [-12, 4, 4, 4, 4, -1, -1, -1, -1].\end{aligned}\quad (17)$$

Since the exact form of the deviation is known, the correction terms are also known exactly and can be set in the following form:

$$\psi_{ji} = \Psi_{ji\alpha} \partial_\alpha P''_{\alpha\kappa}, \quad (18)$$

$$\phi_{ji} = \Phi_{ji} \partial_\alpha (q'_\alpha + q''_\alpha). \quad (19)$$

For an isothermal problem, where the energy equation is not required, by setting the temperature equal to $T = 1/3$, the magnitude of these deviation terms becomes of the order of $O(u^3)$ and can be neglected in most flow applications, as done in the standard isothermal LB method. However, for the present nonisothermal flow, these deviation terms become large enough to influence the simulation results. For this reason, a correction scheme is necessary to eliminate all of the deviation terms and to obtain the correct macroscopic limits.

The full description of the correction terms and the resulting discretized lattice BGK equation is presented in detail in Appendices A and B.

V. VARIABLE PRANDTL NUMBER

Control of the thermal conductivity independently of the dynamic viscosity allows the adjustment of the Prandtl number, $\text{Pr} = \nu/\alpha$ [ratio of the kinematic viscosity $\nu = \mu/\rho$ to the heat diffusivity $\alpha = \kappa/(2C)$]. For that, there exist mainly two solutions. The first is to modify the collision process by introducing another intermediate state or quasiequilibrium similar to Refs. [36,37]. The second, which is also adopted in this paper, is to use and modify the correction scheme of the previous section, similar to Ref. [19]. To this purpose, the following term is added in the energy equation:

$$q_{j\alpha}^{\text{Pr}} = \left(\frac{4}{\text{Pr} \bar{M}} - \frac{4}{M_j} \right) X_j \tau_1 C T \partial_\alpha T, \quad (20)$$

where $\bar{M}$ is the mean molecular weight and Pr is the desired value of the Prandtl number. This correction, combined with the deviation terms mentioned in Sec. IV, generates the final form of the correction terms for the energy equation with adjustable Prandtl number,

$$\phi_{ji} = \Phi_{ji} \partial_\alpha (q'_{j\alpha} + q''_{j\alpha} + q_{j\alpha}^{\text{Pr}}), \quad (21)$$

with the corresponding heat conductivity being

$$\kappa = \frac{2\tau_1 C T}{\text{Pr} \bar{M}}. \quad (22)$$

VI. SIMULATION RESULTS: TRANSPORT COEFFICIENTS

In order to ensure the correct implementation of the theory presented in the previous sections, simulation results are initially presented in three simple setups. Aiming at validating the transport coefficients, namely, the viscosity, conductivity, and mass diffusivity, we examine the transient behavior of the model in (a) the Couette flow (viscosity), (b) the case of heat diffusion over a semi-infinite plane (conductivity), and (c) the binary mass diffusion (mass diffusivity). In all three cases, comparison is done with analytical solutions.

A. Viscosity

Concerning the viscosity values of the proposed model, the Couette flow between two parallel plates is considered. The simulation domain is a Cartesian grid with $N_x = 3$ computational nodes along the x direction (horizontal) and $N_y = 40$ nodes along the y direction (vertical). The bottom plate is moving with velocity $U_x = 0.01$ in LB units along the horizontal axis, while the top plate is stationary. The plates are considered as solid and the diffusive boundary condition is implemented [38]. On the left and right sides of the domain, periodic boundary conditions are applied. The gas mixture is composed of two species, A and B, with molecular weights $M_A = 1$ and $M_B = 8.5$, respectively. The temperature and the species concentration is uniform along the domain, and the mole fraction of species A is $X_A = 20\%$ and of B is $X_B = 80\%$. For this example, the dynamic viscosity of the mixture is set to $\mu = 0.35$ in LB units and the mass diffusivity is $D_{AB} = D_{BA} = 0.08$. The simulation result is shown in Fig. 1. The symbols represent the LB simulation results and the solid continuous line is the analytical solution [39] at three different time instances: (a) after $t_1 = 1000$ time steps, (b) after $t_2 = 3000$ time steps, and (c) at the steady state.

FIG. 1. Couette flow: Comparison of the velocity profile U_x along the y axis calculated by current LB model (symbols) and analytical solution [39] (solid lines), at times $t_1 = 1000$, $t_2 = 3000$, and at the steady state.

B. Heat diffusion

Concerning the heat conductivity of the model, heat conduction in a semi-infinite plane is simulated. The fluid is again a mixture composed of two species. The simulation domain is discretized by $N_x = 200$ computational nodes and $N_y = 3$ nodes, for the x and y directions, respectively. The left boundary of the domain is kept at a constant temperature, T_{Wall} , and heats up the fluid in the rest of the domain, which is initially kept at a lower temperature, $T_\infty = 1/3$. The temperature difference is $\Delta T = T_{Wall} - T_\infty = 0.01 T_\infty$. The molecular weight of species A is $M_A = 1$ and of species B is $M_B = 4$. The mole fractions are $X_A = 20\%$ and $X_B = 80\%$, respectively.

In order to compare LB results with the analytical solution, the heat diffusivity α is treated as constant during the simulation. For the specific example, the kinematic viscosity was set to $\nu = 0.01$ in LB units and $Pr = 0.2$ (which yields $\alpha = 0.05$). The hot wall is modeled with the help of the diffusive boundary condition, while the right boundary of the domain is treated as if it is of infinite length, by copying the distribution functions from the second-to-last node to the last one. The top and bottom boundaries of the domain are periodic boundaries. The simulation result is compared with the analytical solution of this problem [41] at three different instances, $t_1 = 4000$, $t_2 = 10\,000$, and $t_3 = 20\,000$ time steps, as shown in Fig. 2. Notice that this simulation also serves as a validation of the procedure for adjusting the Prandtl number.

C. Mass diffusion of binary mixture

Concerning the mass diffusivity of the model, the mass diffusion of a binary gas mixture is simulated. The simulation domain is discretized by $N_x = 100$ computational nodes and $N_y = 3$ nodes, for the x and y directions, respectively. The domain is divided in two regions, left and right, which contain mixtures of species A and B at equilibrium, held at

FIG. 2. Heat diffusion: Comparison of the temperature profile of current LB model (symbols) and analytical solution of heat diffusion in a semi-infinite plane [40] (solid lines), at times $t_1 = 4000$, $t_2 = 10\,000$, and $t_3 = 20\,000$. ($\Delta T = T_{Wall} - T_\infty = 0.01 T_\infty$, where $T_\infty = 1/3$.)

FIG. 3. Mass diffusion of binary mixture: Comparison of the species' mole fraction profiles of current LB model (symbols) and analytical solution of mass diffusion (solid lines), at times $t_1 = 500$, $t_2 = 3000$ and $t_3 = 10\,000$.

different composition but at the same temperature, $T = 0.4$. The molecular weight of species A is $M_A = 1$ and of species B is $M_B = 7.5$. The mole fraction of the mixture on the left side is $X_A = 60\%$ and $X_B = 40\%$. The right region has a composition of $X_A = 40\%$ and $X_B = 60\%$. At time $t = 0$, the interface separating the two regions is removed and, due to the existence of concentration gradients, mass diffusion and mixing take place.

The simulation result is compared with the existing analytical solution (Fick's second law). The mass diffusivity is set to $D = 0.009$ in LB units and the Schmidt number to $Sc = 0.9$. The left and right boundaries of the domain are treated as infinite by copying the distribution functions from the nodes from the second column to the first, and from the second-to-last column to the last, respectively. The top and bottom sides of the domain are periodic boundaries. The simulation result is compared with the analytical solution of Ref. [41] at three different instances, $t_1 = 500$, $t_2 = 3000$, and $t_3 = 10\,000$ time steps, and is presented in Fig. 3.

For all three setups, the agreement between analytical solutions and LB results is excellent.

VII. COMPARISON WITH OTHER NUMERICAL CODES

In this section, more complicated flows are studied and validation is done with the help of numerical codes. For the first setup, a finite difference numerical tool is used, while for the second setup, we utilize the OPPDIF numerical solver [42].

A. Binary mixing in the presence of temperature gradients

In the first setup, the binary mixing of two species in the presence of temperature gradients is studied. A two-dimensional domain filled with a mixture of two species, A and B , is considered. The molecular weight of species A is $M_A = 1$ g/mol and of species B is $M_B = 4$ g/mol. The domain size is 0.4 m along the x direction and infinitely long

FIG. 4. (Color online) Mixing in the presence of temperature gradients: Comparison of LB simulation results (symbols) with the prediction of the numerical algorithm (solid lines) for (a) $t = 2$ s and (b) $t = 30$ s. Top graphs: The red lines and adjacent filled triangles represent the temperature profiles, and the black lines and open squares represent the velocity along the x axis. In the bottom graphs, the blue lines and adjacent squares represent the mole fraction of gas A and the black lines and the adjacent diamonds are the mole fraction of B.

in the y direction. The domain is divided into two regions, left and right, which contain mixtures of species A and B at equilibrium, held at different temperatures and compositions. The mole fraction of the mixture of the left side is $X_A = 51\%$ and $X_B = 49\%$ at temperature of 360 K. The right region has a composition of $X_A = 49\%$ and $X_B = 51\%$ and is held at a temperature of 840 K. At the same time, the pressure in both regions is considered to be the same in order to avoid the generation of shock waves. At time $t = 0$, the interface dividing the two regions is removed and, given the existence of concentration and temperature gradients, mixing and heat transfer occur simultaneously. The changes in composition affect the heat transfer throughout the domain; conversely, the temperature changes affect the diffusion of species.

The simulation domain is discretized by $N_x = 200$ nodes along the horizontal x axis and $N_y = 3$ nodes along the y direction. The kinematic viscosity of the gas mixture is set as $\nu = \frac{\mu}{\rho} = 1 \times 10^{-5} \text{ m}^2/\text{s}$, the mass diffusivity is $D = 3 \times 10^{-5} \text{ m}^2/\text{s}$, and the Prandtl number is $\text{Pr} = 1$. The left and right boundaries of the domain are treated as infinite by copying the distribution functions from the second-to-last node to the last one. On the top and bottom boundaries, periodic boundary conditions are applied.

Simulation results are compared against the results of an in-house finite difference solver. The 1D code solves for the flow, species, and energy equation. Solution of the flow is obtained using the pressure-correction SIMPLER algorithm [43]. Results are presented in Fig. 4. Comparison is presented between the LB simulation results (symbols) and the prediction of the numerical algorithm (lines) at two different time instances: (a) $t = 2$ s and (b) $t = 30$ s. In the top two graphs of Fig. 4, the red lines and adjacent filled triangles represent the temperature profile, and the black lines and the adjacent open squares represent the velocity along the x axis. In the bottom graphs of Fig. 4, the blue lines and adjacent squares represent the mole fraction of gas A, while the black lines and the diamonds are the mole fraction of B.

It should be noticed that the left side of the domain has lower temperature and therefore higher density compared to the right side. This results in a relatively weak flow that shifts the axis of symmetry of the species and temperature profiles toward the direction of lower density. It is an effect that both codes reproduce. The velocity profile is well captured despite its relatively small magnitude, leading in turn to a very good agreement for the off-symmetry shapes of the species profiles as time evolves.

In Fig. 5, the results of the same simulation setup for different Prandtl number are presented. The time instance $t = 30$ s is plotted. The Prandtl number is set, $\text{Pr} = 8$, while keeping all other parameters the same. The dashed line represents the temperature profile shown in Fig. 5(b) obtained for $\text{Pr} = 1$. The heat diffuses now at a slower rate, as can be seen from the steeper temperature profile, which is the effect of the higher Prandtl number.

FIG. 5. (Color online) Mixing with the presence of temperature gradients: Comparison of the LB simulation results (symbols) with the prediction of the numerical algorithm (line) at time $t = 30$ s. The red solid line and triangles represent the temperature profile for $\text{Pr} = 8$. The black dashed line is the temperature curve of Fig. 4(b) calculated at $t = 30$ s for $\text{Pr} = 1$.

TABLE I. Conditions for two cases of opposed jet flow.

Simulation Case	Jets Side	Velocity (m/s)	Temperature (K)	Mole Fraction	
				O ₂ (%)	H ₂ O(%)
I	Left	1.9	405	60	40
	Right	1.9	495	40	60
II (steep)	Left	0.6	373	10	90
	Right	1.0	3357	90	10

B. Opposed jet flow

In this section, the opposed jet flow setup is considered. Two opposite jets with different composition and temperature flow against each other. Mass, momentum, and heat transfer take place at the same time. Due to its complexity, there are no analytical solutions available for this setup. The comparison of the LB results is done against the OPPDIF code, which is a well-documented numerical tool, developed at Sandia National Laboratories. OPPDIF is a one-dimensional code that takes advantage of the self-similarity present in this flow configuration. Details concerning this algorithm, which is primarily used in multicomponent chemically reacting applications, can be found in Ref. [42].

The fluid flow is generated by two different jet streams impinging against each other through the left and right nozzles and exiting through the top and bottom outlets. The distance between the two nozzles is 0.1 cm. The two jets have different gas concentrations, velocities, and temperatures. Both streams are composed of water vapor, H₂O, and oxygen, O₂. A stagnation plane is established in between the jets at the final steady state. The location of the stagnation plane as well as the temperature, concentration, and velocity distribution of the flow field at the steady state solely depend on the inlet flow conditions.

Two simulations under different conditions are considered, as shown in Table I. For case II, the concentration and temperature difference between the two streams is set to create very steep gradients.

The domain is discretized by $N_x \times N_y = 100 \times 200$ grid points. The two nozzles are located at $X = 0$ and $X = 0.1$ cm and the inlets are located in the y axis, as shown in Fig. 6. The inlet boundary conditions are applied by imposing the equilibrium populations that correspond to the desired inlet velocity, concentration, and temperature. The nodes on the boundaries along the y axis that are not inlet nodes are treated as solid walls. The rest of the boundary domain on the y axis is treated as a stationary wall by imposing zero velocity and the same temperature and concentration as the inflow. On the top and bottom outlet boundaries, zero-Neumann boundary conditions are implemented by copying the populations from the neighboring nodes found in the inner domain.

For the simulation setup of case I (see Figs. 6 and 7), the kinematic viscosity is $\nu_I = 3 \times 10^{-5}$ m²/s, the mass diffusivity is $D_I = 5 \times 10^{-5}$ m²/s, and the Prandtl number is $Pr_I = 0.3$. The results along the plane of vertical symmetry at $Y = 0.1$ cm are plotted in Fig. 7. Symbols represent the temperature, mole fraction, and velocity values of the LB result. The continuous lines represent the predictions of OPPDIF.

FIG. 6. (Color online) Opposed jet flow: The temperature contour and velocity vector field of case II. Two jet streams enter the domain from the left and right inlet (left and right sides). The outflow of the gas mixture is on the top and bottom of the domain.

For the simulation setup of case II, the temperature and concentration gradients are much steeper than case I. The ratio of temperatures between the two jets is set to be nine. The kinematic viscosity is $\nu_{II} = 1 \times 10^{-5}$ m²/s, the mass diffusivity is $D_{II} = 3 \times 10^{-6}$ m²/s, and the Prandtl number is $Pr_{II} = 3$. In Fig. 8, the comparison between LB simulation results (symbols) and OPPDIF predictions (solid lines) is

FIG. 7. (Color online) Opposed jet flow: Case I. Comparison between the LB simulation results (symbols) and the OPPDIF predictions (solid lines). Top: the red line and adjacent triangles represent the temperature profiles; the black line and squares represent the velocity magnitude along the x direction. Bottom: the blue line and squares represent the H₂O mole fraction; the black line and diamonds represent the mole fraction of O₂.

FIG. 8. (Color online) Opposed jet flow: Case II. Comparison between the LB simulation results (symbols) and the OPPDIF predictions (solid lines). Top: the red line and adjacent triangles represent the temperature profile; the black line and squares represent the velocity magnitude along the x direction. Bottom: the blue line and adjacent squares represent H_2O mole fraction; the black line and diamonds represent the mole fraction of O_2 .

presented. The agreement is excellent for all relevant fields: mole fractions, temperature profiles, and velocity profiles. This setup reveals that the model is numerically stable, accurate, and can handle large temperature variation conditions that are common in reactive flows and combustion.

VIII. CONCLUSIONS

A two-dimensional lattice Boltzmann model, suitable for simulation of thermal flows that involve binary mixtures, has been derived, analyzed, and tested in detail. The model combines the properties and advantages of (a) a recently proposed thermal single-component model and (b) a recently proposed multicomponent isothermal model. The proper macroscopic limit is guaranteed, using a correction scheme that removes all deviation of the model from the desired macroscopic set of equations. The resulting model can handle large density gradients, concentration gradients, and temperature gradients. The energy equation includes several important terms, among others, the enthalpy flux due to relative motion of the mixture. The model has the flexibility to independently set the Prandtl, Schmidt, and, therefore, Lewis number. Simulation results for several benchmark cases reveal excellent agreement with analytic solutions (whenever they exist) and simulation results of other numerical computational fluid dynamics (CFD) codes.

The aforementioned qualities suggest that the model can be used for simulating a multitude of applications, *inter alia* the simulation of reactive flows in small energy conversion units or for the study of processes in fuel cell systems. Its extension to three dimensions ($D3Q27$) and the inclusion of more species is straightforward.

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APPENDIX A: MACROSCOPIC LIMIT

The macroscopic limit of this model is derived via the Chapman-Enskog analysis. The equilibrium higher order moments for species j (index j can be A or B and is not a repeated index) are

$$\begin{aligned}
 P_{j\alpha\beta}^{eq} &= P_{j\alpha\beta}^{MB} = C_j T \delta_{\alpha\beta} + \frac{\rho_j J_\alpha J_\beta}{\rho^2}, \\
 Q_{j\alpha\beta\gamma}^{eq} &= Q_{j\alpha\beta\gamma}^{MB} + Q'_{j\alpha\beta\gamma} = C_j T \left(\frac{J_\alpha}{\rho} \delta_{\beta\gamma} + \frac{J_\beta}{\rho} \delta_{\alpha\gamma} + \frac{J_\gamma}{\rho} \delta_{\alpha\beta} \right) \\
 &\quad + \frac{\rho_j J_\alpha J_\beta J_\gamma}{\rho^3} + Q'_{j\alpha\beta\gamma}, \\
 q_{j\alpha}^{eq} &= q_{j\alpha}^{MB} + q'_{j\alpha} = Y_j J_\alpha \left(\frac{J^2}{\rho^2} + \frac{4T}{M_j} \right) + q'_{j\alpha}, \\
 R_{j\alpha\beta}^{eq} &= R_{j\alpha\beta}^{MB} + R'_{j\alpha\beta} = C_j RT \left(\frac{J^2}{\rho^2} + \frac{4T}{M_j} \right) \delta_{\alpha\beta} \\
 &\quad + \frac{\rho_j J_\alpha J_\beta}{\rho^2} \left(\frac{6T}{M_j} + \frac{J^2}{\rho^2} \right) + R'_{j\alpha\beta}, \tag{A1}
 \end{aligned}$$

where $Q'_{j\alpha\beta\gamma}$, $q'_{j\alpha}$, and $R'_{j\alpha\beta}$ are the deviations of the higher order moments from the kinetic theory [Maxwell Boltzmann form (MB)]. These deviations can be calculated exactly and their form is

$$\begin{aligned}
 q'_{j\alpha} &= \frac{1-3T}{M_j} Y_j J_\alpha - \frac{Y_j J_\alpha^3}{\rho^2}, \quad Q'_{j\alpha\alpha\alpha} = Q'_{j\alpha\alpha\alpha} = 0, \\
 Q'_{j\alpha\alpha\alpha} &= \frac{1-3T}{M_j} Y_j J_\alpha - \frac{Y_j J_\alpha^3}{\rho^2}, \quad Q'_{j\alpha\alpha\alpha} = \frac{1-3T}{M_j} Y_j J_\alpha - \frac{Y_j J_\alpha^3}{\rho^2}, \\
 R'_{j\alpha\beta} &= (2-6T) \frac{C_j J_\alpha J_\beta}{\rho^2} - \frac{Y_j J_\alpha J_\beta J^2}{\rho^3}, \tag{A2} \\
 R'_{j\alpha\alpha} &= \frac{1-3T}{M_j} C_j T + \frac{(1-6T)C_j J_\alpha^2}{\rho^2} + \frac{Y_j J_\alpha^4}{\rho^3}, \\
 R'_{j\alpha\beta} &= \frac{1-3T}{M_j} C_j T + \frac{(1-6T)C_j J_\alpha^2}{\rho^2} + \frac{Y_j J_\alpha^4}{\rho^3}.
 \end{aligned}$$

1. Macroscopic momentum equation and viscosity

The mixture viscosity at the macroscopic limit can be derived by studying the mass and momentum equation. The nonequilibrium pressure tensor $P_{\alpha\beta}^{(neq)}$ is found to be

$$\begin{aligned}
 P_{\alpha\beta}^{(neq)} &= -\tau_1 C T \partial_\gamma \left(\frac{J_\alpha}{\rho} \delta_{\beta\gamma} + \frac{J_\beta}{\rho} \delta_{\alpha\gamma} - \frac{J_\gamma}{\rho} \delta_{\alpha\beta} \right) \\
 &\quad + P''_{\alpha\beta}, \tag{A3}
 \end{aligned}$$

where $P''_{\alpha\beta} = -\tau_1 \partial_\gamma Q'_{\alpha\beta\gamma} + \frac{\tau_1}{2} \partial_\gamma q'_{\alpha\beta}$ is the deviation term of $P_{\alpha\beta}^{(neq)}$ and is given at the end of this section. The macroscopic momentum

equation can then be written as follows:

$$\partial_t J_\alpha + \partial_\alpha P + \partial_\beta \left[\frac{J_\alpha J_\beta}{\rho} - \tau_1 CT \partial_\gamma \left(\frac{J_\alpha}{\rho} \delta_{\beta\gamma} + \frac{J_\beta}{\rho} \delta_{\alpha\gamma} - \frac{J_\gamma}{\rho} \delta_{\alpha\beta} \right) \right] + \partial_\beta P''_{\alpha\beta} = 0. \quad (\text{A4})$$

The viscosity for the gas mixture is identified as $\mu = \tau_1 CT$, and the term $\partial_\beta P''_{\alpha\beta}$ is the resulting deviation from the continuum Navier-Stokes equations that has to be removed. It is the sum of the deviation caused by components A and B such that $\partial_\beta P''_{\alpha\beta} = \partial_\beta P''_{A\alpha\beta} + \partial_\beta P''_{B\alpha\beta}$. The specific form of the deviation for species $j = A$ or B , for the x and y direction, are

$$\partial_\beta P''_{jx\beta} = -\partial_x \left\{ \tau_1 \partial_x \left(\frac{1-3T}{M_j} Y_j J_x - \frac{Y_j J_x^3}{\rho^2} \right) - \frac{\tau_1 X_j}{2} \left[\partial_x \left(\frac{1-3T}{M} J_x - \frac{J_x^3}{\rho^2} \right) + \partial_y \left(\frac{1-3T}{M} J_y - \frac{J_y^3}{\rho^2} \right) \right] \right\}, \quad (\text{A5a})$$

$$\partial_\beta P''_{jy\beta} = -\partial_y \left\{ \tau_1 \partial_y \left(\frac{1-3T}{M_j} Y_j J_y - \frac{Y_j J_y^3}{\rho^2} \right) - \frac{\tau_1 X_j}{2} \left[\partial_x \left(\frac{1-3T}{M} J_x - \frac{J_x^3}{\rho^2} \right) + \partial_y \left(\frac{1-3T}{M} J_y - \frac{J_y^3}{\rho^2} \right) \right] \right\}. \quad (\text{A5b})$$

2. Macroscopic energy equation and heat conductivity

Similar analysis leads to the derivation of the macroscopic energy equation of the bare model. The nonequilibrium contracted third order moment is found to be

$$q''_\alpha = -\tau_1 \left[4CT \sum_j^{A,B} \frac{X_j}{M_j} \partial_\alpha T - \frac{4T}{\tau_1} \sum_j^{A,B} \frac{V_{j\alpha}}{M_j} \right] + q''_\alpha, \quad (\text{A6})$$

where q''_α is the deviation term of $q_\alpha^{(neq)}$ and is given in detail at the end of this section.

The recovered macroscopic equation for the evolution of temperature reads

$$\begin{aligned} \partial_t T = & -T \partial_\alpha u_\alpha - u_\alpha \partial_\alpha T + \frac{1}{C} \partial_\alpha \left(2\tau_1 CT \sum_j \frac{X_j}{M_j} \partial_\alpha T \right) - \frac{1}{C} \nabla \cdot \left(\sum_{j=1}^N 2T C_j \mathbf{U}_j \right) \\ & + \frac{1}{C} \tau_1 CT \partial_\alpha u_\beta (\partial_\alpha u_\beta + \partial_\beta u_\alpha - \partial_\gamma u_\gamma \delta_{\alpha\beta}) - \frac{1}{2C} \partial_\alpha (q'_\alpha + q''_\alpha), \end{aligned} \quad (\text{A7})$$

where the last term on the right-hand side is the deviation of the bare LB model from the desired macroscopic limit. The deviation of the energy equation contains the terms $\partial_\alpha q'_\alpha$ and $\partial_\alpha q''_\alpha$. The former is given in Eq. (A2) and the latter is $\partial_\alpha q''_\alpha = \partial_\alpha q''_{A\alpha} + \partial_\alpha q''_{B\alpha}$, where

$$q''_{j\alpha} = \frac{3\tau_1 C_j T}{M_j} \partial_\alpha T + \frac{\tau_2 (1-3T)}{M_j} [Y_j \partial_\alpha P - \partial_\alpha (X_j P)] + \tau_1 \left\{ \begin{aligned} & -\frac{3Y_j J_\alpha^2}{\rho^2} \partial_\alpha P - \frac{3X_j P J_\alpha}{\rho} \partial_\beta \frac{J_\beta}{\rho} + \frac{3X_j C_j J_\alpha J_\beta}{2\rho^2} \partial_\beta T \\ & - (1-3T) \partial_\beta \frac{X_j C_j J_\alpha J_\beta}{\rho^2} + \frac{X_j (1-3T) J_\alpha}{2\rho} \partial_\beta \frac{J_\beta}{M} \\ & + \partial_\alpha \frac{C_j J_\alpha^2}{\rho^2} - \partial_\beta \frac{Y_j J_\beta J_\alpha^3}{\rho^3} - \frac{X_j J_\alpha}{2\rho} \partial_\beta \frac{J_\beta^3}{\rho^2} - \partial_\alpha \frac{Y_j J_\alpha^4}{\rho^3} + \partial_\beta \frac{Y_j J_\alpha J_\beta J^2}{\rho^3} \end{aligned} \right\},$$

where index j indicates species A or B , and index α indicates the direction and can be x or y . In the above Eq. (A8), Einstein summation is assumed only for the repeated index β .

At this point, it is useful to note that only the first terms of Eq. (A8) are large enough to influence the simulation results in usual flow cases. Thus, many of the deviation terms can be neglected, simplifying the scheme. Of course, for a fully Galilean invariant scheme, all deviation terms must be neutralized.

APPENDIX B: DISCRETIZED LB EQUATION AND NUMERICAL SCHEME

Due to the different characteristic velocities of each species given by Eq. (2), the spatial discretization is different in comparison to the single-component LB model. For the numerical implementation of the present multicomponent

model, the interpolation strategy which was studied and presented in detail in Ref. [34] is followed. The basis lattice accommodates exactly the lighter species, i.e., the one with the largest characteristic velocity. The heavier species is propagating off-lattice and an interpolation process is used to distribute the populations on the lighter species lattice nodes.

The discretization of the kinetic equation (16) follows, as usual, the trapezoidal rule and is done similarly to Refs. [19,27,44]. The following transformation of variables is implemented:

$$\begin{aligned} g_{ji} = & f_{ji} + \frac{\delta t}{2\tau_1} [f_{ji} - f_{ji}^*] + \frac{\delta t}{2\tau_2} [f_{ji}^* - f_{ji}^{eq}] \\ & - \frac{\delta t}{2} [\phi_{ji} + \varphi_{ji}], \end{aligned} \quad (\text{B1})$$

and the resulting discretized evolution equation can be written as

$$g_{ji}(t + \delta t) = g_{ji}(t) - \frac{2\delta t}{\delta t + 2\tau_1} [g_{ji}(t) - f_{ji}^*(t)] - \frac{2\delta t}{\delta t + 2\tau_1} \frac{\tau_1}{\tau_2} [f_{ji}^*(t) - f_{ji}^{eq}(t)] + \frac{2\tau_1\delta t}{\delta t + 2\tau_1} [\psi_{ji}(t) + \phi_{ji}(t)]. \quad (\text{B2})$$

For the usual scheme, $\delta t = 1$. The higher order moments of the transformed populations g_{ji} are related to the populations f_{ji} with the help of Eq. (B1). For the local density, momentum, and temperature, respectively,

$$\rho_j(f) = \rho_j(g), \quad (\text{B3a})$$

$$J_{j\alpha}(f) = \frac{J_{j\alpha}(g) + \frac{\delta t}{2\tau_2} J_{j\alpha}^{eq}(f) + \frac{\delta t}{2} \sum_{i=0}^8 c_{ji\alpha} \psi_{ij}}{(1 + \frac{\delta t}{2\tau_2})}, \quad (\text{B3b})$$

$$T(f) = \frac{E(f) - \frac{J(f)^2}{\rho(f)}}{2C} = \frac{E(g) - \frac{J(g)^2}{\rho(g)}}{2C} + \frac{\delta t}{4C} \sum_{i=0, j}^{i=8, j=A, B} c^2 \phi_{ij}. \quad (\text{B3c})$$

For the simulations presented in this paper, the correction terms have been calculated using a second order accurate finite difference scheme, similar to Ref. [19].

APPENDIX C: TRANSFORMATION OF UNITS

In order to connect LB units with physical units, a proper transformation is needed. As usual, the dimensionless numbers that describe the flow have to be the same. For this paper,

the relevant dimensionless numbers are the Reynolds number (Re), Prandtl number (Pr), and Schmidt number (Sc). First we determine L' , which is the correspondence between the characteristic length of the physical system L and the discretized lattice characteristic length L_{LB} (number of grid points),

$$L' = L/L_{LB}. \quad (\text{C1})$$

The next step is to choose a characteristic velocity and then scale the viscosity ν in a way that the flows in both systems are characterized by the same Reynolds number. For example, for the opposed jet flow, we relate the constant inlet velocity U to the LB one, U_{LB} . This, in turn, gives a unique matching parameter for the scaling of real ν to LB viscosity ν_{LB} ,

$$U' = U/U_{LB}, \quad \nu' = \nu/\nu_{LB} = L'U'. \quad (\text{C2})$$

The scaling for the thermal diffusivity and mass diffusivity is done in the same way in order to guarantee the equivalence between the physical and the LB system values for $\text{Pr} = \nu/\alpha$ and $\text{Sc} = \nu/D$. The physical units of viscosity ν_{LB} , thermal diffusivity α_{LB} , and mass diffusivity D_{LB} are the same, therefore,

$$D' = D/D_{LB} = L'U', \quad \alpha' = \alpha/\alpha_{LB} = L'U'. \quad (\text{C3})$$

The scaling factor for temperature T , pressure P , and concentration C are chosen such that the ideal gas law $P = CRT$ is satisfied,

$$P' = P/P_{LB}, \quad T' = T/T_{LB}, \quad \text{and} \quad C' = \frac{P'}{R'T'}, \quad (\text{C4})$$

where the gas constant is $R = 8.314 \text{ J/mol K}$, and its corresponding value in LB units is $R_{LB} = 1$.

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