MRT discrete Boltzmann modeling of multicomponent mixture with nonequilibrium effects

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(Dated: February 10, 2020)
Abstract

A multiple-relaxation-time discrete Boltzmann model (DBM) is proposed for multicomponent mixtures, where compressible, hydrodynamic, and thermodynamic nonequilibrium effects are taken into account. It allows the specific heat ratio and the Prandtl number to be adjustable, and is suitable for both low and high speed fluid flows. From the physical side, besides being consistent with the multicomponent Navier-Stokes equations, Fick’s law and Stefan-Maxwell diffusion equation in the hydrodynamic limit, the DBM provides more kinetic information about the nonequilibrium effects. The physical capability of DBM to describe the nonequilibrium flows, beyond the Navier-Stokes representation, enables the study of the entropy production mechanism in complex flows, especially in multicomponent mixtures. Moreover, the current kinetic model is employed to investigate the compressible nonequilibrium Kelvin-Helmholtz instability (KHI). It is found that, in the dynamic KHI process, the mixing degree and fluid flow are similar for cases with various thermal conductivity and initial temperature configurations. Physically, both heat conduction and temperature exert slight influences on the formation and evolution of the KHI.

PACS numbers: 47.11.-j, 47.20.Ft, 51.10.+y

I. INTRODUCTION

Numerical simulations of multicomponent mixtures with essential nonequilibrium characteristics are of great importance in many fields of science and engineering [1–3], as these practical systems are often too complex to be studied by experiment or theory in a simple and intuitive way. A typical case is the spacecraft reentry into the atmosphere under the condition of low air density and high flight speed [3]. Other typical examples include the porous media bio-filtration device, micro electro-mechanical system, microfluidic device, geological storage of nuclear wastes, carbon dioxide sequestration, combustion chamber, and rotating detonation propulsion engine. For such phenomena where thermodynamic nonequilibrium effect (TNE) has a significant role due to the small characteristic length and/or sharp physical gradient, the traditional continuous description usually breaks down [4–6]. To resolve this issue, the computational kinetic theory is sought as a promising approach. As

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a central equation in the kinetic theory, the Boltzmann equation has the capability to describe complex fluid flows with both hydrodynaminc and thermodynamic nonequilibrium effects. However, in practice, it is usually too complicated to be employed for simulations in a straightforward way. Consequently, various kinetic models based on a simplified and/or discretized Boltzmann equation are proposed [7–12]. In the evolution of the discrete Boltzmann equation, the particle velocity space is discretized besides the discretization in physical space. The physical variables are calculated from the discrete distribution functions whose evolution is obtained with proper numerical methods.

The lattice Boltzmann method (LBM), developed from the lattice gas method and originally based on the discrete Boltzmann equations [1], has been successfully used as an alternative tool of various partial differential equations for complex systems with multi-phase [13–16], multi-component [17,19], mass diffusion [20, 21], external force [22], and/or chemical reactions [23, 24], etc. In 2012, Makhija et al. utilized a multiple-relaxation-time (MRT) LBM, with independent control of Reynolds and Schmidt numbers, to predict the multicomponent flow [17]. In 2016, Liang et al. employed an MRT multiphase LBM to investigate the three-dimensional (3-D) Rayleigh-Taylor instability in a long square duct [14]. In 2019, Chai et al. presented an MRT LBM, as a solver of the Stefan-Maxwell continuum equations, for the mass diffusion in multicomponent mixtures [20]. Although the LBM has achieved great success in replacing traditional continuum governing equations, few of the lattice Boltzmann models could provide various significant thermodynamic nonequilibrium information beyond the continuum equations.

To address this problem, one possible method is to modify the lattice Boltzmann equation by introducing an artificial discrete equilibrium distribution function that satisfies higher order kinetic moments [25]. However, the artificial term becomes particularly complicated with increasing kinetic moments required [25]. In fact, a more direct way is to invoke a novel methodology, the discrete Boltzmann method (DBM), which is regarded as a modern variant of the standard LBM [26–38]. The DBM does not belong to the family of classic LBM solvers. Standard LBMs mainly serve as solvers of (incompressible) Navier-Stokes (NS) equations or other partial differential equations and aim to be loyal to these original equations. The DBM is equivalent to a modified hydrodynamic model plus a coarse-grained model of the thermodynamic nonequilibrium behaviors [26–38]. To be specific, the DBM kinetic modeling goes beyond traditional macroscopic governing equations in terms of physics recovered. The
The numerical scheme adopted for the DBM is just a compromise between the physical gain and computational cost.

Due to its solid physical foundation, the DBM has been applied to investigate various complex fluid flows and gained some new physical insights into the corresponding systems, including multiphase flows [26, 27], reactive flows [29, 32], and fluid instabilities [33, 36]. Besides theoretical analyses and experimental data [31], DBM results have been confirmed and supplemented by numerical solutions of molecular dynamics [4, 5], direct simulation Monte Carlo [6], etc. Generally, in terms of relaxation time, the DBM can be divided into two classes, single-relaxation-time (SRT) DBM [6, 26, 32, 34] and MRT DBM [28, 36–38]. From the perspective of fluid species, it can be classified into two categories, single-component DBM [26, 33] and multi-component DBM [28, 31, 32, 35]. Now, we propose a first MRT DBM for multicomponent flows. Compared with SRT DBMs where there is only one relaxation time and a fixed Prandtl number $\text{Pr} = 1$ [26, 27, 32], the MRT DBM has various relaxation times for different nonequilibrium processes and a flexible $\text{Pr}$. In contrast to single-component DBMs [26, 33], it is also suitable for physical systems where the interaction between different fluid components is of great importance. As a preliminary application, the current model is used to study the nonequilibrium mixing process induced by the Kelvin-Helmholtz instability (KHI) in this work.

The KHI is a fundamental interfacial instability in fluid mechanics [39]. It occurs when there is velocity shear across a wrinkled interface in a fluid system, and leads to the formation of vortices and turbulence [39]. KHI phenomena are ubiquitous in nature and are of considerable interest in scientific and engineering fields [40–45]. Although the KHI has been investigated extensively, there are still some open problems, such as the effect of heat conduction or ablation, on which the conclusion is highly controversial [40–44]. Viscous potential flow analysis of the KHI around a liquid-vapor interface suggests that heat transfer (resulting in mass transfer) tends to enhance the unstable process of a fluid system [40, 41]. On the contrary, comparison of numerical results between the classical and ablative KHIs indicates that thermal conduction (with dissipative nature) stabilizes the flow by impeding the linear growth rate and frequency, suppressing the perturbation transmission and fine structures, but it promotes the vortex pairing process and large-scale structures [42, 43]. Very recently, Gan et al. proposed an easily implementable DBM for the KHI with flexible specific-heat ratio and Prandtl number, and found that the thermal conduction firstly
restrains then strengthens the KHI afterwards because it extends both density and velocity transition layers simultaneously.

However, the aforementioned studies on KHI are based on numerical models only applicable to single-component fluids where a heavy (light) medium has a low (high) temperature. It is worth emphasizing that, for such a situation, changes of density and temperature are strongly coupled due to the equation of state. In other words, the heat transfer always results in mass transfer, and vice versa. For the sake of investigating an independent thermal effect on KHI, it is necessary to adopt a two-component (or multicomponent) physical model suitable for the practical situation where the changes of density and temperature are not blended together. In fact, it is one reason why we develop the MRT DBM for multicomponent mixtures and apply it to the thermal KHI in this research. The rest of the paper is organized as follows. Details of our DBM are described in Sec. II. In Sec. III, the model is validated by three benchmarks, i.e., the three-component diffusion, the thermal Couette flow, and the Sod tube shock. Then, the DBM is employed to investigate the compressible nonequilibrium KHI with various initial temperature and thermal conductivity in Sec. IV. Finally, Sec. V gives conclusions and discussions.

II. DISCRETE BOLTZMANN MODEL

Note that the DBM is a special discretization of the Boltzmann equation in particle velocity space. First of all, let us introduce symbols $f_i^\sigma$ and $\hat{f}_i^\sigma$ which denote the discrete distribution functions in the velocity and moment spaces, respectively, see Eq. (10). Here the subscript $i$ ($= 1, 2, \ldots, N$) represents the number of discrete velocities $v_{i\alpha}^\sigma$, and the total number is $N$ ($= 16$) in this work, see Eq. (20). The superscript $\sigma$ stands for the chemical species in a fluid mixture.

The individual mass density $\rho^\sigma$, molar number density $n^\sigma$, momentum $J_{\alpha}^\sigma$, and velocity $u_{\alpha}^\sigma$ are obtained from the following relations,

$$\rho^\sigma = m^\sigma n^\sigma = m^\sigma \sum_i f_i^\sigma, \quad (1)$$

$$J_{\alpha}^\sigma = \rho^\sigma u_{\alpha}^\sigma = m^\sigma \sum_i f_i^\sigma v_{i\alpha}^\sigma, \quad (2)$$

with the molar mass $m^\sigma$. The mixing mass density $\rho$, number density $n$, momentum $J_{\alpha}$,
and velocity \( u_\alpha \) are given by

\[
\rho = \sum_\sigma \rho^\sigma, \tag{3}
\]

\[
n = \sum_\sigma n^\sigma, \tag{4}
\]

\[
J_\alpha = \rho u_\alpha = \sum_\sigma J_\alpha^\sigma. \tag{5}
\]

The individual and mixing energies are, respectively,

\[
E^\sigma = \frac{1}{2} \sum_i f_i^\sigma (v_i^2 + \eta_i^2), \tag{6}
\]

\[
E = \sum_\sigma E^\sigma, \tag{7}
\]

where \( \eta_i \) corresponds to rovibrational energies corresponding to molecular rotation and/or vibration.

The individual and average temperatures are, respectively,

\[
T^\sigma = \frac{2E^\sigma - \rho^\sigma u^\sigma_2}{(D + I^\sigma)n^\sigma}, \tag{8}
\]

\[
T = \frac{2E - \rho u^2}{\sum_\sigma (D + I^\sigma)n^\sigma}, \tag{9}
\]

where \( D = 2 \) and \( I^\sigma \) indicates rovibrational degrees of freedom.

Furthermore, let us introduce two kinds of discrete equilibrium distribution functions in the velocity and moment spaces, respectively. The first sets are \( f_i^{\sigma\text{eq}} \) and \( \hat{f}_i^{\sigma\text{eq}} \) which are functions of \( (n^\sigma, u_\alpha, T) \) (see Appendix A). The second ones are \( f_i^{\sigma\text{seq}} \) and \( \hat{f}_i^{\sigma\text{seq}} \) that depend upon \( (n^\sigma, u^\sigma_\alpha, T^\sigma) \), and their expression are given by substituting \( (n^\sigma, u^\sigma_\alpha, T^\sigma) \) for \( (n^\sigma, u_\alpha, T) \) in formulas of \( f_i^{\sigma\text{eq}} \) and \( \hat{f}_i^{\sigma\text{eq}} \), respectively (see Appendix A). The projection of discrete (equilibrium) distribution functions from velocity onto moment spaces is

\[
\hat{f}^\sigma = M^\sigma f^\sigma, \tag{10}
\]

\[
\hat{f}^{\sigma\text{eq}} = M^\sigma f^{\sigma\text{eq}}, \tag{11}
\]

\[
\hat{f}^{\sigma\text{seq}} = M^\sigma f^{\sigma\text{seq}}, \tag{12}
\]

in terms of the column matrices

\[
f^\sigma = \left( f_1^\sigma f_2^\sigma \ldots f_N^\sigma \right)^T, \tag{13}
\]

\[
\hat{f}^\sigma = \left( \hat{f}_1^\sigma \hat{f}_2^\sigma \ldots \hat{f}_N^\sigma \right)^T. \tag{14}
\]
The discrete Boltzmann equations take the form,

\[ \partial_t f^\sigma_i + v^\sigma_{i\alpha} \partial_\alpha f^\sigma_i = -M^{-1} S_{ik} \left( \hat{f}_{k}^\sigma - \hat{f}_{k}^{\sigma_{eq}} \right) + A_i^\sigma. \]  

On the left-hand side, \( t \) is the time, \( \alpha = x, y \) the physical space for a 2-D system. On the right-hand side, \( S_{ik}^\sigma \) is the element of a diagonal matrix \( S^\sigma = \text{diag}(S_1^\sigma, S_2^\sigma, \ldots, S_N^\sigma) \), and the parameter \( S_i^\sigma \) controls the relaxation speed of \( \hat{f}_i^\sigma \) approaching \( \hat{f}_{i}^{\sigma_{eq}} \). \( M^{-1}_{il} \) is the element of the square matrix \( M^{-1} \) which is the inverse of \( M^\sigma \) with the element \( M_{il}^\sigma \) (see Appendix A). \( A_i^\sigma \) is an additional term expressed by Eqs. (21) and (22).

As shown in Fig. 1, the discrete velocities read

\[ \left( v_x^\sigma, v_y^\sigma \right) = \begin{cases} v_a^\sigma \left( \cos \frac{i\pi}{8}, \sin \frac{i\pi}{8} \right) & \text{for } 1 \leq i \leq 8, \\ v_b^\sigma \left( \cos \frac{i\pi}{8}, \sin \frac{i\pi}{8} \right) & \text{for } 9 \leq i \leq N. \end{cases} \]  

Besides, we define \( \eta_i^\sigma = \eta_a^\sigma \) for \( 1 \leq i \leq 4 \), and \( \eta_i^\sigma = \eta_b^\sigma \) for \( 9 \leq i \leq 12 \), otherwise, \( \eta_i^\sigma = 0 \). Here \( v_a^\sigma, v_b^\sigma, \eta_a^\sigma, \) and \( \eta_b^\sigma \) are flexible parameters. It is worth mentioning that these parameters

\[ \begin{align*} 
\mathbf{f}^{\sigma_{eq}} &= \begin{pmatrix} f_1^{\sigma_{eq}} & f_2^{\sigma_{eq}} & \cdots & f_N^{\sigma_{eq}} \end{pmatrix}^T, \\
\hat{\mathbf{f}}^{\sigma_{eq}} &= \begin{pmatrix} \hat{f}_1^{\sigma_{eq}} & \hat{f}_2^{\sigma_{eq}} & \cdots & \hat{f}_N^{\sigma_{eq}} \end{pmatrix}^T, \\
\mathbf{f}^{\sigma_{seq}} &= \begin{pmatrix} f_1^{\sigma_{seq}} & f_2^{\sigma_{seq}} & \cdots & f_N^{\sigma_{seq}} \end{pmatrix}^T, \\
\hat{\mathbf{f}}^{\sigma_{seq}} &= \begin{pmatrix} \hat{f}_1^{\sigma_{seq}} & \hat{f}_2^{\sigma_{seq}} & \cdots & \hat{f}_N^{\sigma_{seq}} \end{pmatrix}^T. 
\end{align*} \]
can be adjusted to optimize the DBM properties. (I) The conditions \( \nu_{\alpha}^\sigma \neq \nu_{\beta}^\sigma \neq 0 \) and \( \eta_{\alpha}^\sigma \neq \eta_{\beta}^\sigma \neq 0 \) should be satisfied to ensure the matrix \( \bf{M}^\sigma \) invertible. (II) For the sake of numerical stability, the sizes of \( v_{\alpha}^\sigma \) and \( v_{\beta}^\sigma \) should be around the values of flow velocity \( \bf{u}^\sigma \) and sound speed \( \nu_{\sigma}^\sigma = \sqrt{\gamma^\sigma T^\sigma / m^\sigma} \), where \( \gamma^\sigma \) denotes the specific heat ratio. (III) The values of \( \eta_{\alpha}^\sigma \) and \( \eta_{\beta}^\sigma \) should be around the value of \( \sqrt{I^\sigma T^\sigma / m^\sigma} \), because the extral internal energy is \( \frac{1}{2}m^\sigma \nu_{\sigma}^2 = \frac{1}{2}I^\sigma T^\sigma \) in the local thermodynamic equilibrium according to the equipartition of energy theorem.

It is noteworthy that, to ensure consistency with traditional NS equations in the hydrodynamic limit (see Appendix B), an additional term \( A_i^\sigma \) is imposed on the right-hand side of Eq. (19). To be specific, \( A_i^\sigma = 0 \) for \( 1 \leq i \leq 7 \) and \( 10 \leq i \leq 16 \), and

\[
\hat{A}_8^\sigma = 2 (S_8^\sigma - S_8^\sigma) u_x^\sigma \Delta_5^\sigma + 2 (S_8^\sigma - S_6^\sigma) u_y^\sigma \Delta_6^\sigma, \tag{21}
\]

\[
\hat{A}_9^\sigma = 2 (S_9^\sigma - S_7^\sigma) u_x^\sigma \Delta_7^\sigma + 2 (S_9^\sigma - S_6^\sigma) u_y^\sigma \Delta_6^\sigma, \tag{22}
\]

in terms of

\[
\Delta_5^\sigma = \frac{2n^\sigma T^\sigma}{S_5^\sigma m^\sigma} \left( \frac{1 - D - I^\sigma}{D + I^\sigma} \partial_x u_x^\sigma + \frac{\partial_y u_y^\sigma}{D + I^\sigma} \right), \tag{23}
\]

\[
\Delta_6^\sigma = -\frac{n^\sigma T^\sigma}{S_6^\sigma m^\sigma} (\partial_y u_x^\sigma + \partial_x u_y^\sigma), \tag{24}
\]

\[
\Delta_7^\sigma = \frac{2n^\sigma T^\sigma}{S_7^\sigma m^\sigma} \left( \frac{\partial_x u_x^\sigma}{D + I^\sigma} + \frac{1 - D - I^\sigma}{D + I^\sigma} \partial_y u_y^\sigma \right). \tag{25}
\]

In addition, the Fick’s laws of diffusion and Stefan-Maxwell diffusion equation could also be derived from the multicomponent NS equations under corresponding assumptions (see Appendix C).

Besides giving abovementioned continuum equations, the DBM also provides a set of handy, effective and efficient tools to describe and probe the abundant kinetic information beyond them. Let us define \( \hat{f}_i^\sigma = \hat{f}_{i \text{seq}} + \hat{f}_{i \text{neq}} \), with the equilibrium part \( \hat{f}_{i \text{seq}} \) and nonequilibrium part \( \hat{f}_{i \text{neq}} \), respectively. (It is the reason why Eq. (12) is introduced. In a similar way, we can define \( \hat{f}_i^\sigma = \hat{f}_{i \text{eq}} + \hat{f}_{i \text{neq}} \)). Concretely, \( \hat{f}_{i \text{seq}} = 0 \) for \( 1 \leq i \leq 4 \) in line with conservation laws, as \( \hat{f}_i^\sigma = \hat{f}_{i \text{seq}} = n^\sigma, J_x^\sigma / m^\sigma, J_y^\sigma / m^\sigma, 2E^\sigma / m^\sigma \) for \( i = 1, 2, 3, 4 \), respectively. In contrast, the nonequilibrium quantity \( \hat{f}_{i \text{neq}} \) may not equal zero for \( 5 \leq i \leq 16 \) in a nonequilibrium state. Physically, \( \hat{f}_{i \text{neq}} \) denotes the departure of a kinetic mode \( \hat{f}_i^\sigma \) from its equilibrium counterpart \( \hat{f}_{i \text{seq}} \). The speed of relaxation process from \( \hat{f}_i^\sigma \) to \( \hat{f}_{i \text{seq}} \) is controlled by the relaxation parameter \( S_{i}^\sigma \), and both \( \hat{f}_{i \text{seq}} \) and \( S_{i}^\sigma \) exert influence on
the thermodynamic and hydrodynamic behaviours. Simultaneously, various nonequilibrium
effects interplay with each other, and these kinetic modes are coupled as well. For instance,
at the NS level,
\[
\hat{f}_{\sigma s\text{neq}}^{5} = \Delta_{5}^{\sigma} - n^{\sigma} \left( u_{\sigma x}^{2} - u_{\sigma y}^{2} \right) + \frac{2 S_{5}^{\sigma} n^{\sigma}}{S_{5}^{\sigma}} u_{\sigma x}^{\sigma} \left( u_{\sigma x}^{\sigma} - u_{\sigma x} \right) - \frac{S_{4}^{\sigma} n^{\sigma} \left( u_{\sigma x}^{\sigma} - u_{\sigma}\right)^{2} + \left( u_{\sigma y}^{\sigma} - u_{\sigma y} \right)^{2}}{D + I_{\sigma}} + \left( S_{4}^{\sigma} - S_{5}^{\sigma} \right) n^{\sigma} \frac{T^{\sigma} - T}{S_{5}^{\sigma} m^{\sigma}},
\]
(26)
\[
\hat{f}_{\sigma s\text{neq}}^{6} = \Delta_{6}^{\sigma} - n^{\sigma} \left( u_{\sigma x}^{\sigma} u_{\sigma y}^{\sigma} - u_{\sigma x} u_{\sigma y} \right) + \frac{S_{5}^{\sigma} n^{\sigma}}{S_{6}^{\sigma}} u_{\sigma y}^{\sigma} \left( u_{\sigma x}^{\sigma} - u_{\sigma x} \right) - \frac{S_{3}^{\sigma} n^{\sigma} \left( u_{\sigma y}^{\sigma} - u_{\sigma y} \right)^{2}}{D + I_{\sigma}} + \left( S_{4}^{\sigma} - S_{5}^{\sigma} \right) n^{\sigma} \frac{T^{\sigma} - T}{S_{5}^{\sigma} m^{\sigma}},
\]
(27)
\[
\hat{f}_{\sigma s\text{neq}}^{7} = \Delta_{7}^{\sigma} - n^{\sigma} \left( u_{\sigma y}^{2} - u_{\sigma y}^{2} \right) + \frac{S_{7}^{\sigma} n^{\sigma} u_{\sigma y}^{\sigma} \left( u_{\sigma y}^{\sigma} - u_{\sigma y} \right)}{S_{7}^{\sigma}} - \frac{S_{4}^{\sigma} n^{\sigma} \left( u_{\sigma x}^{\sigma} - u_{\sigma x} \right)^{2} + \left( u_{\sigma y}^{\sigma} - u_{\sigma y} \right)^{2}}{D + I_{\sigma}} + \left( S_{4}^{\sigma} - S_{7}^{\sigma} \right) n^{\sigma} \frac{T^{\sigma} - T}{S_{7}^{\sigma} m^{\sigma}},
\]
(28)
which are derived from the Chapman-Enskog analysis, reduce to \( \hat{f}_{\sigma s\text{neq}} \), \( \hat{f}_{\sigma s\text{neq}}^{5} = \Delta_{5}^{\sigma} \), \( \hat{f}_{\sigma s\text{neq}}^{6} = \Delta_{6}^{\sigma} \), and \( \hat{f}_{\sigma s\text{neq}}^{7} = \Delta_{7}^{\sigma} \) under conditions of \( u_{\sigma}^{\alpha} = u_{\alpha} \) and \( T^{\sigma} = T \).

The above mentioned capability of this DBM makes convenient to study behaviors in the
nonequilibrium process, such as the entropy production \([27, 30, 45]\). Especially, with \( X^{\sigma} \) the molar fraction of species \( \sigma \), the entropy of mixing,
\[
S_{M} = - \sum_{\sigma} n^{\sigma} \ln X^{\sigma},
\]
which is part of the increasing entropy as separate mixable fluids contact and mix, can be
obtained in each iterative step.

It should be stressed that kinetic effects are significant and traditional hydrodynamic
models are not sufficient for fluid flows with small characteristic scales or large Knudsen
numbers \([26, 38]\). The TNE becomes crucial and even dominant in the evolution of multicomponent flows due to the existence of various complex material and/or mechanical interfaces \([26, 38]\). In such complicated cases, to investigate the TNE is a significant and
convenient way to study the fundamental kinetic processes. Making convenient such studies
is the objective of discrete Boltzmann modeling.

In addition, the DBM has the advantage of simplicity for coding and high efficiency
of parallel processing, since the set of formulas in Eq. \((19)\) are uniformly linear and the
information transfer in DBM is local in both time and space \[45\]. Actually, the parallel programming based on the Message-Passing Interface are used for all simulations in this work. Moreover, we adopt the second-order nonoscillatory and nonfree-parameter dissipation difference scheme to deal with the space derivatives \([46]\) and the second-order Runge-Kutta method to treat the time derivative in Eq. \([19]\). Note that the current Runge-Kutta method is an explicit scheme, so the temporal step should be no greater than the minimum of the relaxation times \(\tau_m\) in order to have accurate and robust solutions. To be specific, it is necessary to satisfy the relation \(\Delta t \leq \tau_m\), where \(\tau_m = \min \left(S_i^{\sigma-1} \right)\) is the minimum of the reciprocal of \(S_i^\sigma\) with \(i = 1, 2, \ldots, N\).

III. VERIFICATION AND VALIDATION

For practical calculations, it is convenient and useful to use dimensionless variables. In this work, physical quantities are expressed in nondimensional forms using the following references, i.e., the molar mass \(m_0\), molar number density \(n_0\), length \(L_0\), temperature \(T_0\), and universal gas constant \(R\). For example,

| Dimensionless Variables | By |
|-------------------------|-----|
| Distribution functions: \(f_i^\sigma\) | \(n_0\) |
| Mass density: \(\rho^\sigma, \rho\) | \(m_0n_0\) |
| Speed and velocity: \(v_s^\sigma, \eta_i^\sigma, u^\sigma, u\) | \(\sqrt{RT_0/m_0}\) |
| Energy density: \(E^\sigma, E\) | \(n_0RT_0\) |
| Pressure: \(p^\sigma, p\) | \(n_0RT_0\) |
| Temperature: \(T^\sigma, T\) | \(T_0\) |
| Coordinate: \(x, y\) | \(L_0\) |
| Time: \(t\) | \(L_0/\sqrt{RT_0/m_0}\) |

In the following are three subsections. The first part is for the three-component diffusion, which is to demonstrate the capacity of the present DBM in dealing with the interaction among various nonpremixed chemical species. The second subsection is to use the thermal Couette flow to validate that our DBM is suitable for fluid flows where both Prandtl number and specific heat ratio are flexible. Finally, the Sod shock tube is simulated to show that this model has the capability of describing the shock wave with a high Mach number (as well as the rarefaction wave).
A. Three-component diffusion

Diffusion is the net movement of molecules driven by a gradient in chemical potential of fluid species \([1, 47]\). As one of the most important and fundamental transport processes, it has received great attention due to its significance in chemical process and biological engineering \([1, 2, 47]\), etc.

To demonstrate that the DBM could describe the interaction among various chemical species, we carry out the simulation of multicomponent diffusion. As shown in Fig. 2, the initial configuration is

\[
\begin{array}{c|c}
L_0 & \\
\hline
n^A = 0.80 & n^A = 0.20 \\
n^B = 0.15 & n^B = 0.60 \\
n^C = 0.05 & n^C = 0.20 \\
\end{array}
\]

where the subscripts \(L\) and \(R\) indicate \(0 < x \leq L_0/2\) and \(L_0/2 < x \leq L_0\), respectively, with \(L_0 = 0.1\). The superscripts \(A\), \(B\), and \(C\) represent three chemical species, respectively. For simplicity, the molar mass is chosen as \(m^σ = 1\). The average velocity and temperature are \(u = 0\) and \(T = 1\). The pressure on the two sides equals \(p = 1\), hence the interface remains rest. In the horizontal direction the quantities on the ghost nodes outside the boundary are replaced by the neighbouring ones \([48, 49]\), while the boundary conditions are periodic in the vertical direction. In fact, this case is a 1-D problem as the physical field is the same in the \(y\) direction. Hence, the mesh is chosen as \(N_x \times N_y = N_x \times 1\). The spatial step is \(\Delta x = \Delta y = L_0/N_x\), the temporal step \(\Delta t = 4 \times 10^{-4}\), the relaxation parameters \(S_i = 10^3\), the rovibrational degrees of freedom \(I^σ = 3\), and the parameters \((\nu_a^σ, \nu_b^σ, \eta_a^σ, \eta_b^σ) = (0.01, 2, 2.7, 2.55)\).

First of all, let us perform a grid convergence analysis, which is an important issue for numerical models. To this end, we carried out some simulations under various spatial steps.
FIG. 3. Grid convergence analysis: (a) the horizontal distribution of mole fractions $X^A$ at the time $t = 0.05$, (b) relative errors under various spatial steps.

$\Delta x_1 = L_0/10$, $\Delta x_2 = L_0/20$, $\Delta x_3 = L_0/40$, and $\Delta x_4 = L_0/80$, respectively. Figure 3 (a) shows the mole fraction of species $A$. The long-dashed, short-dashed, dash-dotted and short-dotted lines stand for DBM results under $\Delta x_1$, $\Delta x_2$, $\Delta x_3$, and $\Delta x_4$, respectively. The solid line denotes the analytical solution (1, 47),

$$X^\sigma = \frac{X^\sigma_L + X^\sigma_R}{2} - \frac{X^\sigma_L - X^\sigma_R}{2} \text{Erf} \left( \frac{x - x_0}{\sqrt{4Dt}} \right), \quad (31)$$

where Erf is the complementary error function, $x_0 = L_0/2$ is the location of the interface, $D = 10^{-3}$ is the diffusivity. It can be found that, with decreasing spatial steps (i.e., increasing resolution), the numerical results converge towards the analytical solution. Particularly, the results with spatial step $\Delta x_4$ are quite close to the solution, which is satisfactory.

For the purpose of a quantitative analysis, Fig. 3 (b) gives relative errors versus spatial steps. The relative error takes the form

$$\text{Error}(\phi) = \sqrt{\frac{\sum_{(x,y)} |\phi_a(x, y, t) - \phi_n(x, y, t)|^2}{\sum_{(x,y)} |\phi_a(x, y, t)|^2}} \quad (32)$$

where $\phi_a$ and $\phi_n$ denote the analytical and numerical results of the variable $\phi$ (e.g., the mole fraction $X^A$). The circles represent the DBM results and the line stand for the fitting function, $\ln(\text{Error}) = 2.079 \ln(\Delta x) + 7.6887$. Clearly, the slope of the fitting function is close to 2.0, which indicates that the current model has a second-order convergence rate in space.

Figure 4 illustrates molar fractions, $X^\sigma = n^\sigma/n$, at various times in the diffusion process. The spatial step is $\Delta x_4$, which is validated in Fig. 3 (a). Symbols denote numerical results at various times $t = 0.005$ (squares), 0.02 (circles), 0.06 (triangles), and 0.2 (diamonds),
FIG. 4. Molar fractions in the diffusion process: $X^A$ (top), $X^B$ (middle), and $X^C$ (bottom). Squares, circles, triangles, and diamonds denote DBM results at time constants $t = 0.005, 0.02, 0.06, \text{ and } 0.2$, respectively. Solid lines stand for the corresponding analytical solutions.

respectively. Lines denote the analytical solutions. It is evident that the DBM results coincide with the analytical solutions in the evolution of the diffusion.

Moreover, to further validate that the DBM has the capability of capturing nonequilibrium effects, Fig. 5 plots nonequilibrium quantities $\hat{f}_5^{\text{eq}}$ at time $t = 0.02$ in the diffusion process. Symbols represent our DBM results, and lines represent the analytical solutions in Eq. (26). Obviously, our simulation results are in excellent agreement with the analytical solutions. Consequently, it is confirmed that the DBM can be used to probe and measure nonequilibrium manifestations.
FIG. 5. Nonequilibrium quantities at time $t = 0.02$ in the diffusion process. Squares, circles, and triangles denote DBM results of $f_5^{A_{neq}}$, $f_5^{B_{neq}}$, and $f_5^{C_{neq}}$, respectively. Solid lines stand for the corresponding analytical solutions.

\[ u = u_0 e_x \]

\[
\begin{align*}
  n^A &= 0.1 \\
  n^B &= 0.3 \\
  n^C &= 0.6 \\
  T_0 &= 1 \\
  H &= \text{distance}
\end{align*}
\]

FIG. 6. Initial configuration of the thermal Couette flow.

B. Thermal Couette flow

In fluid dynamics, thermal Couette flow is the flow of a viscous fluid between two surfaces with relative shear movement. It is a classical benchmark to test a model for compressible fluid flows where viscosity and heat transfer dominate \cite{50,51}. Here we conduct simulations of the thermal Couette flow for two purposes. One aim is to verify that the DBM is suitable for various values of the specific heat ratio $\gamma$ and Prandtl number $\text{Pr}$. The other aim is to verify the DBM for the case with premixed compressible fluid species.

Figure 6 delineates the sketch of initial configuration for this problem. A premixed fluid flow with species, $\sigma = A, B, C$, is between two infinite parallel flat plates separated by a distance $H$. The concentrations are $(n^A, n^B, n^C) = (0.1, 0.3, 0.6)$, the molar mass $m_\sigma = 1$, the temperature $T_\sigma = 1$, and the velocity $u_\sigma = 0$. The upper plate moves horizontally at the
\[
\begin{array}{cccccc}
\text{Cases} & \text{Pr} & \sigma & S_{i=5,6,7} & S_{i\neq 5,6,7} & I^\sigma \\
\hline
\text{Run I} & 1.0 & 1.3 & 1000 & 1000 & 14/3 \\
\text{Run II} & 1.0 & 1.4 & 1000 & 1000 & 3 \\
\text{Run III} & 1.0 & 1.5 & 1000 & 1000 & 2 \\
\text{Run IV} & 0.5 & 1.4 & 2000 & 1000 & 3 \\
\text{Run V} & 2.0 & 1.4 & 500 & 1000 & 3 \\
\end{array}
\]

TABLE I. Parameters for the thermal Couette flow.

FIG. 7. Vertical distribution of the horizontal speed \( u_x \) (a) and nonequilibrium quantity \( \hat{f}_{6}^{Asneq} \) (b) in the thermal Couette flow. Squares, circles, triangles, and diamonds represent DBM results at time constants \( t = 0.1, t = 0.4, t = 2.0, \) and \( t = 30 \), respectively. Solid lines stand for the corresponding analytical solutions.

speed \( u_0 = 0.1 \), while the lower plate keeps motionless. The nonequilibrium extrapolation scheme is imposed on the top and bottom, respectively [52]. Periodic boundary conditions are applied for the left and right boundaries, respectively. Because the field is the same in the \( y \) direction, the configuration is actually a 1-D case. The mesh is chosen as \( N_x \times N_y = 1 \times 200 \), the spatial step \( \Delta x = \Delta y = 5 \times 10^{-4} \), the temporal step \( \Delta t = 2 \times 10^{-5} \), the parameters \( (v_a^\sigma, v_b^\sigma, \eta_a^\sigma, \eta_b^\sigma) = (1.5, 1.8, 1.6, 2.5) \), and the remaining parameters are listed in Table II.
Five cases are under consideration with various values of the specific heat ratio and Prandtl number in Table I. In the current DBM, the specific heat ratio of species $\sigma$ takes the form $\gamma^\sigma = (4 + I^\sigma)/(2 + I^\sigma)$, and the Prandtl number of species $\sigma$ is $\Pr^\sigma = S^\sigma_\kappa / S^\sigma_\mu$ under the conditions $S^\sigma_\mu = S^\sigma_5 = S^\sigma_6 = S^\sigma_7$ and $S^\sigma_\kappa = S^\sigma_8 = S^\sigma_9$. Consequently, in terms of $I^\sigma$, $S^\sigma_{i=5,6,7}$ and $S^\sigma_{i=8,9}$, we set $\Pr = 1.0$ and $\gamma = 1.3, 1.4, 1.5$ for Runs I, II, and III, respectively. While the parameters are $\gamma = 1.4$ and $\Pr = 0.5, 1.0, 2.0$ for Runs II, IV, and V, respectively.

Firstly, we consider the case of Run IV in Table I. Figure 7 (a) exhibits the comparisons between the numerical and analytical results of the horizontal speed along the $y$ axis at various time constants. Symbols represent numerical results, and lines represent the following analytical solutions [39, 53],

$$u = \frac{y}{H} u_0 + \frac{2}{\pi} u_0 \sum_{n=1}^{\infty} \frac{(-1)^n}{n} \exp \left( -\frac{n^2 \pi^2 \mu t}{\rho H^2} \right) \sin \left( \frac{n \pi y}{H} \right),$$

where $\mu$ is the viscosity coefficient. Clearly, we can find a good agreement between them in the evolution of the thermal Couette flow. To further demonstrate its capability of measuring nonequilibrium manifestations, Fig. 7 (b) plots the vertical distribution of the nonequilibrium quantity $\tilde{f}^\sigma_{\text{neq}}$ of species $\sigma = A$. Via the Chapman-Enskog analysis, we can obtain the analytical solution in Eq. (27). Obviously, the DBM results are consistent with the analytical solution in the thermal Couette flow.

Figure 8 shows the vertical distribution of the temperature when the thermal Couette flow achieves its steady state. In theory, the analytical solution reads [39, 53],

$$T = T_0 + \frac{\Pr}{2c_p} u_0^2 \frac{y}{H} \left( 1 - \frac{y}{H} \right),$$

where $T_0$ is the temperature of the top/bottom wall, $c_p = \gamma c_v$ the specific heat at constant pressure, $c_v$ the specific heat at constant volume. Temperature depends upon the specific heat ratio and Prandtl number. Figure 8 (a) is for the cases with fixed $\Pr = 1.0$ and various $\gamma = 1.3, 1.4, 1.5$, respectively. Figure 8 (b) is for the cases with fixed $\gamma = 1.4$ and various $\Pr = 0.5, 1.0, 2.0$, respectively. It is clear that simulation results match the corresponding analytical solutions for all cases.
FIG. 8. Vertical distribution of the temperature in steady Couette flow. (a) Cases with $Pr = 1.0$ and $\gamma = 1.3, 1.4, \text{ and } 1.5$, respectively. (b) Cases with $\gamma = 1.4$ and $Pr = 0.5, 1.0, \text{ and } 2.0$, respectively.

C. Sod shock tube

To verify the DBM for high-speed compressible flows, we consider a typical benchmark, the Sod shock tube that includes abundant and complex characteristic structures [54]. It is worth mentioning that, compared with single-component models, the current DBM is applicable to the Sod shock tube that contains various species (with different molar mass and/or specific-heat ratios, etc.) in different locations. As shown in Fig. [10], the initial field reads,

\[
\begin{aligned}
\left\{ \begin{array}{l}
(n^A, n^B, n^C, p)_L = (1.25, 0, 0, 1), \\
(n^A, n^B, n^C, p)_R = (0, 0.0625, 0.0521, 0.1),
\end{array} \right.
\end{aligned}
\]  

(35)

where the subscripts $L$ and $R$ denote the left part $-L_0/2 \leq x < 0$ and right part $0 \leq x < L_0/2$, respectively, with $L_0 = 1.0$. Both parts are initially at rest, i.e. $u = 0$. The molar mass is $(m^A, m^B, m^C) = (0.8, 1, 1.2)$. Consequently, it is easy to obtain $(\rho_L, \rho_R) = (1, 0.125)$ and $(T_L, T_R) = (0.8, 0.87273)$ in terms of $\rho = \sum_{\sigma} m^\sigma n^\sigma$ and $T = p/\sum_{\sigma} n^\sigma$. The specific-heat
ratios are \((\gamma^A, \gamma^B, \gamma^C) = (1.4, 1.5, 1.5)\), and the parameters \((\nu_a^\sigma, \nu_b^\sigma, \eta_a^\sigma, \eta_a^\tau) = (1.5, 3.3, 1.1, 3.9)\). The boundary conditions are the same with those in Fig. 4.

As numerical accuracy and robustness should be under consideration, we carry out simulations of the Sod shock tube with various spatial and temporal steps. Figure 10 plots density profiles at a time constant \(t = 0.2\) in the Sod shock tube. In Fig. 10 (a), the dashed, dotted, dash-dotted, and solid lines represents numerical results under spatial steps \(\Delta x_1 = 4 \times 10^{-3}\), \(\Delta x_2 = 2 \times 10^{-3}\), \(\Delta x_3 = 10^{-3}\), and \(\Delta x_4 = 5 \times 10^{-4}\), respectively. The corresponding meshes are \(N_x \times N_y = 250 \times 1\), \(500 \times 1\), \(1000 \times 1\), and \(2000 \times 1\), respectively. Besides, in Fig. 10 (b), the dashed, dotted, dash-dotted, and solid lines represents numerical results in cases with temporal steps \(\Delta t_1 = 5 \times 10^{-5}\), \(\Delta t_2 = 2.5 \times 10^{-5}\), \(\Delta t_3 = 1.25 \times 10^{-5}\), and \(\Delta t_4 = 6.25 \times 10^{-6}\), respectively. The inset maps in Figs. 10 (a) and (b) are the enlargements of portions within \(0.186 \leq x \leq 0.195\). It indicates that simulation results start to converge with decreasing spatial and temporal steps. Moreover, it can be found that the spatial step \(\Delta x = 5 \times 10^{-4}\) and temporal step \(2.5 \times 10^{-5}\), which are used in Fig. 11 are small enough to give satisfactory simulation results.

Figure 11 illustrates the density (a), horizontal speed (b), temperature (c), and pressure at a time constant \(t = 0.2\) in the Sod shock tube. Symbols and lines stand for our DBM results and the Riemann solutions, respectively. As shown in Figs. 11 (a)-(d), the rarefaction wave (moving leftward), the contact discontinuity (between two media with different concentrations), and the (left-propagating) shock front are captured well. It is clear that the numerical and exact results coincide well with each other.
FIG. 10. Profiles of density at a time constant \( t = 0.2 \) in the Sod shock tube with various spatial steps (a) and temporal steps (b).

FIG. 11. Profiles of density (a), horizontal speed (b), temperature (c), and pressure at a time constant \( t = 0.2 \) in the Sod shock tube. Symbols represent DBM results, and solid lines stand for Riemann solutions.
IV. KELVIN-HELMHOLTZ INSTABILITY

As an essential physical mechanism in turbulence and fluids mixing process, the KHI has been studied extensively with experimental [55–57], theoretical [40, 41, 58], and computational [42–45] methods during the past decades. In this section, we further utilize the DBM to simulate and investigate the compressible KHI with both hydrodynamic and thermodynamic nonequilibrium effects.

Figure 12 portrays the initial configuration for the KHI. The length and height of the calculation domain are \( L_x = 1.5 \) and \( L_y = 0.5 \), respectively. Initially, the left half part is occupied by upward-moving species \( A \) with velocity \( u_L = 0.5e_y \), and the right is filled with \( B \) travelling downwards with velocity \( u_R = -0.5e_y \). To have an initial smooth interface, we impose a transition layer with width \( W = L_x/300 \) on the concentration and velocity fields across the interface. Moreover, to trigger the formation of the KHI, a sinusoidal perturbation, \( w = w_0 \cos(2\pi y/L_y) \), is imposed on the interface with an amplitude \( w_0 = L_x/200 \). The concentration and velocity are expressed by,

\[
\begin{align*}
n &= \frac{n_L+n_R}{2} - \frac{n_L-n_R}{2} \tanh(\frac{x-x_0+w}{W}), \\
u &= \frac{u_L+u_R}{2} - \frac{u_L-u_R}{2} \tanh(\frac{x-x_0+w}{W}),
\end{align*}
\]

where \( x_0 = L_x/2 \) denotes the averaged \( x \) position of the cosine-shaped interface, \( n_L \) and \( n_R \) are the concentrations in the left and right parts, respectively. Across the interface, pressure keeps homogeneous, i.e., \( p_L = p_R \). The two species have an identical velocity and temperature at the same location. In addition, the specular reflection (periodic) boundary condition is used in the \( x \) (\( y \)) direction. The time and space steps are as small as \( \Delta t = 2.5 \times 10^{-5} \) and \( \Delta x = \Delta y = 5 \times 10^{-4} \) to reduce numerical errors. Correspondingly, the mesh is \( N_x \times N_y = 3000 \times 1000 \).
Next, let us study the influence of heat conduction upon the formation and evolution of the nonequilibrium KHI. To this end, ten representative cases are under consideration, see Table II. For the first five cases, the temperatures in the two parts are equal, i.e., $T_L = T_R = 1.0$, the concentrations $n_L = n_R = 1$, the molar mass $m^\sigma = 1$, and the parameters $(v^\sigma_a, v^\sigma_b, \eta^\sigma_a, \eta^\sigma_a) = (2, 3.7, 1.5, 5.5)$. Moreover, the relaxation parameters are $S_8 = S_9 = 1.25 \times 10^3$, $2.5 \times 10^3$, $5.0 \times 10^3$, $1.0 \times 10^4$, and $2.0 \times 10^4$, respectively. The other relaxation parameters are $S_i = 5.0 \times 10^3$. The rovibrational degree of freedom $I^\sigma = 3$.

Actually, in these cases, the initial dynamic viscosity is fixed, and the thermal conductivity is variable, i.e., $\kappa^\sigma = 2.8 \times 10^{-3}, 1.4 \times 10^{-3}, 7.0 \times 10^{-4}, 3.5 \times 10^{-4},$ and $1.75 \times 10^{-4}$, respectively. In other words, the Prandtl number is variable in the five cases. In contrast, for the latter five cases, the temperatures in the two parts are different, namely, $T_L = 1.0$ and $T_R = 2.0$, the molar mass $m^A = 1$ and $m^B = 2$, and the parameters $(v^\sigma_a, v^\sigma_b, \eta^\sigma_a, \eta^\sigma_a) = (1.4, 2.8, 5.0, 2.5)$. The particular thermal conductivity is $(\kappa^A, \kappa^B) = (2.8, 1.4) \times 10^{-3}, (1.4, 0.7) \times 10^{-3}, (7.0, 3.5) \times 10^{-4}, (3.5, 1.75) \times 10^{-4}, (17.5, 8.75) \times 10^{-5}$, respectively. The other parameters in the latter five cases are the same with the former corresponding ones. Additionally, for all above cases, the density is homogeneous, i.e., $\rho = 1$ in the system, hence the Atwood number is a constant $At = (\rho_L - \rho_R)/ (\rho_L + \rho_R) = 0$.

To give an intuitive impression, we take Run I for example and depict the entropy of mix-
FIG. 13. Contours of the entropy of mixing at time constants $t = 0.0, 0.5, 1.0, 1.5, 2.0,$ and $3.0$ in the evolution of KHI.

From top to bottom are its contours at time constants $t = 0.0, 0.5, 1.0, 1.5, 2.0,$ and $3.0$, respectively. It is clear to find a sequence of distinct evolutionary stages, namely, the initial linear growth period, then the nonlinear growth stage, the later time with a highly rolled-up vortice, and finally a turbulent phase with nonregular structures. To be specific, firstly, the smooth interface starts to wiggle due to the initial perturbation and the velocity shear between the two layers. The perturbation grows exponentially and the sinusoidal structure gradually becomes asymmetric. Then, in the nonlinear stage, a braid-shape region is formed and a roughly circular vortex appears. Subsequently, the vortex becomes elliptical with its roll-up movement and it is further stretched in the vertical direction. In the final phase, with the collapse of the normal vortex, the turbulent movements promote the mixing between the two parts until its saturation state.

Figure 14 displays the evolution of physical quantities for the first five cases in Table II. The lines with squares, circles, upper triangles, lower triangles, and diamonds stand for
FIG. 14. Physical quantities in the evolution of KHI with \( T_L = T_R \): (a) the entropy of mixing and its growth rate, (b) the mixing area and its growth rate, (c) the mixing width and its growth rate, (d) the kinetic energy, (e) the internal energy, (f) the total energy, (g) the maximum temperature, (h) the minimum temperature, (i) the temperature difference. The inserts in (d) and (e) correspond to the rectangles, respectively. The lines with squares, circles, upper triangles, lower triangles, and diamonds indicate Pr = 0.25, 0.5, 1.0, 2.0, and 4.0, respectively. The Prandtl number Pr = 0.25, 0.5, 1.0, 2.0, and 4.0, respectively. Figure 14 (a) shows the whole entropy of mixing \( \int \int S_M dxdy \) and its growth rate. Here the integral is extended over the physical region \( L_x \times L_y \). Figure 14 (b) exhibits the value of \( S_a/(L_xL_y) \) and its growth rate, with the mixing area \( S_a \) where the mass fraction of species A is within the range \( 1\% \leq \lambda^A \leq 99\% \). Figure 14 (c) gives the value of \( L_M/L_x \) and its growth rate. Here the mixing width \( L_M \) is defined as the horizontal distance between the leftmost and rightmost points within the region \( 1\% \leq \lambda^A \leq 99\% \). It is clear in Figs. 14 (a)-(c) that the mixing degree, area, and width coincide well with each other in the five cases.

With the definition of the kinetic energy \( E_k = \frac{1}{2} \rho |\mathbf{u}|^2 \), Fig. 14(d) plots the whole kinetic energy \( \int \int E_k dxdy \). With the introduction of the internal energy \( E_i = \frac{1}{2} \sum \sigma (D + I^\sigma)n^\sigma T \),
we show the whole internal energy \( \int \int E_i dxdy \) and its growth rate in Fig. 14(e). The inserts in Figs. 14 (d) and (e) are enlargements of the portions in the corresponding rectangles. It can be found that the kinetic and internal energies in the five cases are almost the same with each other, and their differences are very small. The kinetic (internal) energy becomes only a little larger (smaller) with the increasing Prandtl number, i.e., the decreasing thermal conductivity. Figure 14(f) plots the whole energy \( \int \int E dxdy \) in terms of \( E = E_k + E_i \). It is evident that the energy is a conserved quantity in the KHI process. For instance, in the first case, our DBM gives \( \int \int E dxdy = \int \int E_k dxdy + \int \int E_i dxdy = 0.0883230 + 1.8798020 \) at the time \( t = 3 \), which equals its initial result \( \int \int E dxdy = 0.0931250 + 1.8750000 \). It is noteworthy that, apart from the energy conservation, the mass and momentum conservation is ensured by the DBM as well (which is not shown here).

Figures 14 (g)-(i) are for the maximum temperature \( T_{\text{max}} \), the minimum temperature \( T_{\text{min}} \), and their difference \( T_d = T_{\text{max}} - T_{\text{min}} \). On the whole, the maximum temperature is smaller for larger thermal conductivity. The minimum temperature with various Prandtl numbers competes with each other before the time \( t = 1.5 \), afterwards it is larger for larger thermal conductivity. Hence, the temperature difference becomes smaller with the increasing thermal conductivity that facilitates heat exchange.

Figure 15 exhibits the evolution of physical quantities for the latter five cases in Table II. In the following, comparison is made between Figs. 14 and 15. The former is for the cases in an initial homogeneous temperature field, while the latter initially has a temperature difference between the left and right half parts of the physical domain. Some findings are listed as follows.

(I) From Figs. 14 (a)-(c) and Figs. 15 (a)-(c), it is apparent that the whole entropy of mixing, the mixing area, the mixing width, and their growth rates for various Prandtl numbers basically coincide with each other. That is to say, the heat conduction has a weak effect on the formation and evolution of the KHI for the parameter range here we considered.

(II) It can be found in Figs. 14 (d)-(e) and Figs. 15 (d)-(e) that, the kinetic and internal energies have slight differences for various Prandtl numbers. The inserts show that, for either \( T_L = T_R \) or \( T_L \neq T_R \), the kinetic (internal) energy becomes only a bit smaller (larger) with the reducing Prandtl number, i.e., the increasing thermal conductivity.

(III) The energy conservation is held in the DBM simulation, which is validated in Fig. 14(f) and Fig. 15(f). Take Run X in Table II for instance, the simulation result remains
FIG. 15. Physical quantities in the evolution of KHI with $T_L \neq T_R$: (a) the entropy of mixing and its growth rate, (b) the mixing area and its growth rate, (c) the mixing width and its growth rate, (d) the kinetic energy, (e) the internal energy, (f) the total energy, (g) the maximum temperature, (h) the minimum temperature, (i) the temperature difference. The inserts in (d) and (e) correspond to the rectangles, respectively. The lines with squares, circles, upper triangles, lower triangles, and diamonds indicate Pr = 0.25, 0.5, 1.0, 2.0, and 4.0, respectively.

\[ \int \int E \, dx \, dy = 1.96813, \] which is exactly equal to its exact solution 1.96813. Actually, the mass and momentum conservation is also obeyed by the DBM (which is not shown here).

(IV) Comparison between Figs. 14 (g)-(i) and Figs. 15 (g)-(i) shows that the maximum and minimum temperatures and their differences for $T_L = T_R$ are quite different from those for $T_L \neq T_R$. In Figs. 14 (g)-(i), both maximum and minimum temperatures, and their differences on the whole are larger for a larger thermal conductivity.

(V) Although the evolutionary temperature fields are quite different for various Prandtl numbers, the mixing process is almost the same for homogeneous or inhomogeneous initial temperature configuration. Consequently, the temperature plays a nonessential role in the formation and evolution of the KHI.
FIG. 16. Comparison of physical fields at the time \( t = 1.5 \) in the KHI process. From top to bottom are the mass fraction of species \( A \), vorticity, and temperature in the three rows, respectively. From left to right are the cases \( T_L = T_R \) and \( \text{Pr} = 0.25 \), \( T_L = T_R \) and \( \text{Pr} = 4.0 \), \( T_L \neq T_R \) and \( \text{Pr} = 0.25 \), and \( T_L \neq T_R \) and \( \text{Pr} = 4.0 \) in the four columns, respectively. Only a part of horizontal range \( 0.5 \leq x \leq 1.0 \) is shown in each subfigure.

Finally, for the sake of validating above conclusions again, let us compare the specific KHI fields in four representative cases, i.e., Run I \( (T_L = T_R \text{ and } \text{Pr} = 0.25) \), Run V \( (T_L = T_R \text{ and } \text{Pr} = 2.0) \), Run VI \( (T_L \neq T_R \text{ and } \text{Pr} = 0.25) \), and Run X \( (T_L \neq T_R \text{ and } \text{Pr} = 2.0) \), respectively. Figure 16 depict the contours of physical fields at a time constant \( t = 1.5 \) in the KHI process. The four cases are shown from left to right columns, respectively. The mass fraction \( (\lambda^A) \), the vorticity \( (\omega = \partial_x u_y - \partial_y u_x) \), and the temperature \( (T) \) are plotted from top to bottom rows, respectively. Only a part of the physical domain \( 0.5 \leq x \leq 1.0 \)
and $0 \leq y \leq 0.5$ is shown in each subfigure. Obviously, the fields of mass fraction and vorticity are almost the same (with negligible differences) for all cases. Their shapes and sizes are very similar, despite few differences of the vorticity maxima and minima in the four cases. On the contrary, the contours of temperature fields are similar for the same initial configurations, and are distinguishable for different initial configurations. It is further confirmed that neither temperature nor thermal conductivity has a strong influence on the mass fraction and vorticity in the KHI process. From the point of view of mixing state (such as mixing area and degree) and flow state (including the vortex shapes and sizes), the temperature and thermal conductivity play inessential roles in the spatio-temporal evolution of the KHI.

V. CONCLUSIONS AND DISCUSSIONS

We presented an MRT DBM for compressible multicomponent mixtures with both hydrodynamic and thermodynamic nonequilibrium effects. Physically, the DBM formulation is not only consistent with the NS equations, Fick’s law and Stefan-Maxwell diffusion equation under corresponding conditions in the continuum limit, but also provides more detailed kinetic thermodynamic nonequilibrium information. Such a capability of the DBM, beyond the macroscopic modeling based on the continuum assumption, allows the study of nonequilibrium processes like the entropy production. Mathematically, a set of uniform discrete Boltzmann equations are used to describe multicomponent mixtures, and the linear form of evolution equations makes it easy to code. Computationally, it can be implemented on massively parallel clusters with excellent scalability because all information transfer in DBM is local in time and space.

In addition, several prototype problems, including the three-component diffusion, thermal Couette flow, and Sod shock tube, are simulated to verify and validate the model. It is demonstrated that the present DBM is suitable for both low and high speed compressible nonequilibrium flows, with premixed or nonpremixed chemical species, whose specific heat ratio and Prandtl number are adjustable. Various detailed TNEs in complex fluid flows can be captured, measured, and predicted effectively by the current versatile kinetic model.

Furthermore, the current model is utilized to investigate the compressible KHI with TNEs. Ten cases with various values of thermal conductivity and initial temperature config-
urations are compared and analyzed. It is found that the mixing state (such as the mixing area and degree) and flow state (including the vortex shapes and sizes) are quite similar for all cases in the dynamic KHI process, although the temperature is similar for the same initial configurations and is distinguishable for different initial configurations. The whole kinetic (internal) energy becomes only a bit smaller (larger) with the increasing thermal conductivity. It is concluded that both heat conduction and temperature exert slight influences on the formation and evolution of the KHI, which is absolutely different from previous studies [40–44]. It is noteworthy that previous works are based upon physical models suitable for single-component fluids [40–44], while the present research is on the base of our reliable kinetic model for multicomponent mixtures.

Moreover, the temperature field shows different trends in cases with $T_L : T_R = 1 : 1$ and $1 : 2$, where $T_L$ and $T_R$ denote the temperature in the left and right parts of an initial configuration. To be specific, for the initial homogeneous temperature, the maximum temperature is smaller for larger thermal conductivity as a whole, while the minimum temperature with various Prandtl numbers competes with each other in the early stage and is larger for larger thermal conductivity afterwards. For the initial inhomogeneous temperature, both maximum and minimum temperatures, and their differences on the whole are larger for larger thermal conductivity.

**ACKNOWLEDGMENTS**

This work is supported by the Natural Science Foundation of China (NSFC) under Grant Nos. 51806116, 91441120 and 11772064, CAEP Foundation under Grant No. CX2019033, the opening project of State Key Laboratory of Explosion Science and Technology (Beijing Institute of Technology) under Grant No. KFJJ19-01M, and the Natural Science Foundation of Fujian Provinces (under Grant No. 2018J01654). Support from the UK Engineering and Physical Sciences Research Council under the project UK Consortium on Mesoscale Engineering Sciences (UKCOMES) (Grant No. EP/R029598/1) is also gratefully acknowledged.
Appendix A

The square matrix $M^\sigma$ has $16 \times 16$ elements: $M^\sigma_{1i} = 1$, $M^\sigma_{2i} = v^\sigma_{ix}$, $M^\sigma_{3i} = v^\sigma_{iy}$, $M^\sigma_{4i} = v^\sigma_{i2}$, $M^\sigma_{5i} = v^\sigma_{i2}$, $M^\sigma_{6i} = v^\sigma_{ix}v^\sigma_{iy}$, $M^\sigma_{7i} = v^\sigma_{ix}$, $M^\sigma_{8i} = (v^\sigma_2 + \eta^2) v^\sigma_{ix}$, $M^\sigma_{9i} = (v^\sigma_2 + \eta^2) v^\sigma_{iy}$, $M^\sigma_{10i} = v^\sigma_{ix}$, $M^\sigma_{11i} = v^\sigma_{ix}v^\sigma_{iy}$, $M^\sigma_{12i} = v^\sigma_{ix}v^\sigma_{iy}$, $M^\sigma_{13i} = \eta_2$, $M^\sigma_{14i} = (v^\sigma_2 + \eta^2) v^\sigma_{ix}$, $M^\sigma_{15i} = (v^\sigma_2 + \eta^2) v^\sigma_{ix}v^\sigma_{iy}$, $M^\sigma_{16i} = (v^\sigma_2 + \eta^2) v^\sigma_{ix}v^\sigma_{iy}$. The Einstein summation convention is adopted here.

The NS equations of individual species take the form,

$$
\partial_t \rho^\alpha + \partial_\alpha J^\alpha = 0,
$$

\hfill (B1)

$$
\partial_t J^\alpha + \partial_\beta \left( \delta_{\alpha \beta} \rho^\alpha + \rho^\alpha u^\alpha u^\beta + P^\alpha_{\alpha \beta} + U^\alpha_{\alpha \beta} \right) = S^\alpha_{\gamma \alpha \beta} \rho^\gamma (u_\alpha - u_\alpha^\gamma),
$$

\hfill (B2)

$$
\partial_t E^\sigma + \partial_\alpha \left( E^\sigma u^\alpha_{\alpha} + P^\sigma_{\alpha \beta} u^\alpha_{\beta} - \kappa^\sigma \partial_\alpha T^\sigma + u^\beta_\beta P^\sigma_{\alpha \beta} + Y^\sigma_{\alpha} \right) = \frac{1}{2} \xi_4^\sigma \rho^\sigma \left( \frac{(D + I^\sigma) T - T^\sigma}{m^\sigma} - u^2 - u^2 \right),
$$

\hfill (B3)

in terms of

$$
P^\alpha_{\alpha \beta} = \frac{p^\sigma}{S_{p \alpha \beta}} \left( \frac{2\delta_{\alpha \beta}}{D + I^\sigma} \partial_\alpha u^\alpha_{\alpha} - \partial_\beta u^\alpha_{\alpha} - \partial_\alpha u^\beta_{\beta} \right),
$$

\hfill (B4)
\[
U_{\alpha\beta} = \delta_{\alpha\beta} \frac{S_{4} - S_{\rho\alpha\beta}}{S_{\rho\alpha\beta}} \rho^\sigma \frac{T^\sigma - T}{m^\sigma} + \rho^\sigma (u_{\alpha} u_{\beta} - u_{\alpha}^\sigma u_{\beta}^\sigma)
+ \frac{S_{4} - S_{\rho\alpha\beta}}{S_{\rho\alpha\beta}} \rho^\sigma (u_{\alpha}^\sigma u_{\beta} - u_{\alpha} u_{\beta}^\sigma) + \frac{S_{4} - S_{\rho\alpha\beta}}{S_{\rho\alpha\beta}} \rho^\sigma (u_{\alpha}^\sigma u_{\beta} - u_{\alpha} u_{\beta}^\sigma)
- \delta_{\alpha\beta} \frac{S_{4} - S_{\rho\alpha\beta}}{S_{\rho\alpha\beta}} \rho^\sigma u_{\alpha}^2 + u_{\alpha}^\sigma u_{\alpha}^\sigma - 2u_{\alpha}^\sigma u_{\alpha}^\sigma - u_{\alpha}^\sigma u_{\alpha}^\sigma
\]

\[
Y_{\alpha} = -\frac{S_{4} - S_{\rho\alpha\beta}}{S_{\rho\alpha\beta}} \rho^\sigma u_{\alpha}^2 (u_{\beta}^\sigma - u_{\beta})^2 + \frac{S_{4} - S_{\rho\alpha\beta}}{S_{\rho\alpha\beta}} \rho^\sigma u_{\alpha}^\sigma (u_{\sigma}^\sigma - u_{\beta}^\sigma u_{\beta})
+ \frac{\rho^\sigma}{2S_{\rho\alpha\beta}} (S_{4} - S_{\rho\alpha\beta} u_{\alpha}) \left[(D + I^\sigma + 2) \frac{T^\sigma - T}{m^\sigma} + u_{\alpha}^\sigma u_{\alpha} + u_{\alpha}^\sigma + u_{\alpha}^\sigma \right]
+ \frac{S_{4} - S_{\rho\alpha\beta}}{S_{\rho\alpha\beta}} \left[(D + I^\sigma + 2) \frac{T^\sigma - T}{m^\sigma} + u_{\alpha}^\sigma u_{\alpha} + u_{\alpha}^\sigma + u_{\alpha}^\sigma \right],
\]

where \(S_{4} = S_{2}^\sigma, S_{y} = S_{3}^\sigma, S_{p,xx} = S_{5}^\sigma, S_{p,xy} = S_{6}^\sigma, S_{p,yy} = S_{7}^\sigma, S_{r,xx} = S_{8}^\sigma, S_{r,xy} = S_{9}^\sigma, S_{r,yy} = S_{9}^\sigma\). The thermal conductivity is

\[
\kappa_{\sigma} = \frac{D + I^\sigma + 2 \rho^\sigma T^\sigma}{2S_{\rho\alpha\beta} m^\sigma},
\]

which is reduced to

\[
\kappa_{\sigma} = \frac{D + I^\sigma + 2 \rho^\sigma T^\sigma}{2S_{\rho\alpha\beta} m^\sigma},
\]

in the case \(S_{8} = S_{9} = S_{9}^\sigma\). Moreover, if \(S_{8} = S_{9} = S_{7} = S_{\mu}\), Eq. 4 can be rewritten into

\[
P_{\alpha\beta} = \frac{\mu^\sigma}{S_{\rho\alpha\beta}} \left(2D \frac{\partial_{\alpha} u_{\beta}^\sigma - \partial_{\beta} u_{\alpha}^\sigma - \partial_{\alpha} u_{\beta}^\sigma}{D + I^\sigma} \right) - \delta_{\alpha\beta} \frac{\mu^\sigma}{S_{\rho\alpha\beta}} \partial_{\alpha} u_{\beta}^\sigma,
\]

with the dynamic, kinematic, and bulk viscosities

\[
\mu^\sigma = \frac{\mu^\sigma}{S_{\rho\sigma}},
\]

\[
\nu^\sigma = \frac{\mu^\sigma}{\rho^\sigma} = \frac{T^\sigma}{m^\sigma S_{\rho\sigma}},
\]

and

\[
\mu_{B}^\sigma = \mu^\sigma \left(\frac{2}{D} - \frac{2}{D + I^\sigma}\right)
\]

respectively.

The specific heat at constant pressure and volume are, respectively,

\[
c_{p}^\sigma = \frac{D + I^\sigma + 2}{2m^\sigma},
\]

\[
c_{v}^\sigma = \frac{D + I^\sigma}{2m^\sigma},
\]

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hence the specific-heat ratio is
\[ \gamma^\sigma = \frac{c_p^\sigma}{c_v^\sigma} = \frac{D + I^\sigma + 2}{D + I^\sigma}. \] (B15)

The Prandtl number is
\[ \text{Pr}^\sigma = \frac{c_p^\sigma \mu^\sigma}{\kappa^\sigma} = \frac{S_k^\sigma}{S_\mu^\sigma}. \] (B16)

Consequently, both the specific-heat ratio and Prandtl number are flexible.

Furthermore, summing Eqs. (B1)-(B3) over all species \( \sigma \) results in the NS equations describing mixing fluids as bellow,
\[ \partial_t \rho + \partial_\alpha (\rho u_\alpha) = 0, \] (B17)
\[ \partial_t (\rho u_\alpha) + \partial_\beta \sum_\sigma \left( \delta_{\alpha\beta} p^\sigma + \rho^\sigma u_\alpha^\sigma u_\beta^\sigma + P_{\alpha\beta}^\sigma + U_{\alpha\beta}^\sigma \right) = 0, \] (B18)
\[ \partial_t E + \partial_\alpha \sum_\sigma \left( E^\sigma u_\alpha^\sigma + p^\sigma u_\alpha^\sigma - \kappa^\sigma \partial_\alpha T^\sigma + u_\beta^\sigma P_{\alpha\beta}^\sigma + Y_{\alpha}^\sigma \right) = 0, \] (B19)
under the condition of momentum and energy conservation,
\[ \sum_\sigma \rho^\sigma (u_\alpha - u_\alpha^\sigma) = 0, \] (B20)
\[ \sum_\sigma \rho^\sigma \left( \frac{D + I^\sigma T^\sigma - T}{2} \frac{m^\sigma}{m^\sigma} + \frac{u^\sigma_2 - u_2^\sigma}{2} \right) = 0. \] (B21)

Appendix C

In a similar way to previous works [29, 59], it is easy to demonstrate that the NS equations (B1)-(B3) lead to the following diffusion equations.

(I) Fick’s first law
\[ \Phi^\sigma_\alpha = -D^\sigma \partial_\alpha \rho^\sigma, \] (C1)
where \( \Phi^\sigma_\alpha = \rho^\sigma (u_\alpha^\sigma - u_\alpha) \) is the individual diffusion flux of mass in the \( \alpha \) direction, and \( D^\sigma = T/(m^\sigma S_{Ja}^\sigma) \) is the individual diffusivity.

(II) Fick’s second law
\[ \partial_t \lambda^\sigma = D^\sigma \partial_\alpha (\partial_\alpha \lambda^\sigma), \] (C2)
where \( \lambda^\sigma = \rho^\sigma / \rho \) represents the mass fraction.

(III) Stefan-Maxwell diffusion equation
\[ \partial_\alpha X^j = \frac{S_{Ja}^j}{p} \sum_{k \neq j} \frac{\rho^j \rho^k}{\rho} (u_k^\alpha - u_\alpha^\alpha) + \frac{\lambda^j - X^j}{p} \partial_\alpha p, \] (C3)
with the mixing pressure $p = \sum p^\sigma$ and individual pressure $p^\sigma = n^\sigma T^\sigma$. Here the individual temperature

$$T^\sigma = \frac{2E^\sigma - \rho^\sigma u^2}{(D + I^\sigma) n^\sigma}, \quad (C4)$$

relative to the mixing velocity $u_\alpha$ is different from the one relative to the individual velocity $u_\alpha^\sigma$ in Eq. (8).

Additionally, comparing Eq. (C3) with the traditional Stefan-Maxwell diffusion equation

$$\partial_\alpha X^j = \sum_{k=1}^{N_s} X^j X^k_{D^{jk}} (u^k_\alpha - u^j_\alpha) + \frac{\chi^j - X^j}{p} \partial_\alpha p, \quad (C5)$$

we get

$$S^j_{J\alpha} = \frac{\sum_{k=1}^{N_s} X^j X^k_{D^{jk}} (u^k_\alpha - u^j_\alpha)}{\sum_{k=1}^{N_s} \rho^k_p (u^k_\alpha - u^j_\alpha)}, \quad (C6)$$

with $D^{jk}$ the binary diffusivity. With the assumption that the quantity $(u^k_\alpha - u^j_\alpha)$ is of the same order for all $j \neq k$, the above equation is reduced to

$$S^j_{J\alpha} = \frac{\sum_{k=1}^{N_s} X^j X^k_{D^{jk}}}{\sum_{k=1}^{N_s} \rho^k_p} (1 - \lambda^j), \quad (C7)$$

in terms of

$$\bar{D}^j = \left( \sum_{k=1}^{N_s} X^k_{D^{jk}} \right)^{-1} (1 - \lambda^j), \quad (C8)$$

which is the mixture-averaged diffusion coefficient of component $j$ [60].

Note that substituting Eq. (C7) into (B2) may give a result in contradiction to (B20). A solution to this problem is to set $S^\sigma_{J\alpha} = \sum_j S^j_{J\alpha} / N_s$. Namely, the condition of momentum conservation is satisfied if all individual parameters $S^\sigma_{J\alpha}$ are equal to each other [61]. Another solution is to modify the right-hand side of discrete Boltzmann equation (19) [62]. Similarly, a way to overcome the inconsistency between Eqs. (B3) and (B21) is to set $S^\sigma_j$ as the same value, or to add a modified term to Eq. (19). More discussion is out of this paper.

[1] E. L. Cussler, *Diffusion: mass transfer in fluid systems* (Cambridge university press, Cambridge, 2000).
[2] C. K. Law, *Combustion physics* (Cambridge University Press, Cambridge, 2006).

[3] A. Peng, Z. Li, J. Wu, and X. Jiang, Implicit gas-kinetic unified algorithm based on multi-block docking grid for multi-body reentry flows covering all flow regimes, J. Comput. Phys. **327**, 919 (2016).

[4] H. Liu, W. Kang, Q. Zhang, Y. Zhang, H. Duan, and X. T. He, Molecular dynamics simulations of microscopic structure of ultra strong shock waves in dense helium, Front. Phys. **11**, 115206 (2016).

[5] H. Liu, Y. Zhang, W. Kang, P. Zhang, H. Duan, and X. T. He, Molecular dynamics simulation of strong shock waves propagating in dense deuterium, taking into consideration effects of excited electrons, Phys. Rev. E **95**, 023201 (2017).

[6] Y. Zhang, A. Xu, G. Zhang, Z. Chen, and P. Wang, Discrete boltzmann method for non-equilibrium flows: Based on shakhov model, Comput. Phys. Commun. **238**, 50 (2019).

[7] S. Succi, *The Lattice Boltzmann Equation for Fluid Dynamics and Beyond* (Oxford University Press, New York, 2001).

[8] L. Wu, C. White, T. J. Scanlon, J. M. Reese, and Y. Zhang, Deterministic numerical solutions of the boltzmann equation using the fast spectral method, J. Comput. Phys. **250**, 27 (2013).

[9] C. Liu and K. Xu, A unified gas kinetic scheme for continuum and rarefied flows v: Multiscale and multi-component plasma transport, Commun. Comput. Phys. **22**, 1175 (2017).

[10] Y. Zhang, L. Zhu, R. Wang, and Z. Guo, Discrete unified gas kinetic scheme for all knudsen number flows. iii. binary gas mixtures of maxwell molecules, Phys. Rev. E **97**, 053306 (2018).

[11] A. Xu, G. Zhang, Y. Gan, F. Chen, and X. Yu, Lattice boltzmann modeling and simulation of compressible flows, Front. Phys. **7**, 582 (2012).

[12] A. Xu, G. Zhang, and Y. Zhang, Discrete boltzmann modeling of compressible flows, in *Kinetic Theory*, edited by G. Z. Kyzas and A. C. Mitropoulos (IntechOpen, Rijeka, 2018) Chap. 2.

[13] A. Fakhari and T. Lee, Multiple-relaxation-time lattice boltzmann method for immiscible fluids at high reynolds numbers, Phys. Rev. E **87**, 023304 (2013).

[14] H. Liang, B. C. Shi, and Z. H. Chai, Lattice boltzmann modeling of three-phase incompressible flows, Phys. Rev. E **93**, 013308 (2016).

[15] F. Qin, A. Mazloomi Moqaddam, Q. Kang, D. Derome, and J. Carmeliet, Entropic multiple-relaxation-time multirange pseudopotential lattice boltzmann model for two-phase flow, Phys. Fluids **30**, 032104 (2018).
[16] L. Fei, J. Du, K. H. Luo, S. Succi, M. Lauricella, A. Montessori, and Q. Wang, Modeling realistic multiphase flows using a non-orthogonal multiple-relaxation-time lattice boltzmann method, Phys. Fluids 31, 042105 (2019).

[17] D. Makhija, G. Pingen, R. Yang, and K. Maute, Topology optimization of multi-component flows using a multi-relaxation time lattice boltzmann method, Comput. Fluids 67, 104 (2012).

[18] Z. Chai and T. Zhao, A pseudopotential-based multiple-relaxation-time lattice boltzmann model for multicomponent/multiphase flows, Acta Mech. Sin. 28, 983 (2012).

[19] H. Liu, L. Wu, Y. Ba, G. Xi, and Y. Zhang, A lattice boltzmann method for axisymmetric multicomponent flows with high viscosity ratio, J. Comput. Phys. 327, 873 (2016).

[20] Z. Chai, X. Guo, L. Wang, and B. Shi, Maxwell-stefan-theory-based lattice boltzmann model for diffusion in multicomponent mixtures, Phys. Rev. E 99, 023312 (2019).

[21] S. A. Hosseini, N. Darabiha, and D. Thévenin, Lattice boltzmann advection-diffusion model for conjugate heat transfer in heterogeneous media, Int. J. Heat Mass Transfer 132, 906 (2019).

[22] L. Fei, K. H. Luo, C. Lin, and Q. Li, Modeling incompressible thermal flows using a central-moments-based lattice boltzmann method, Int. J. Heat Mass Transfer 120, 624 (2018).

[23] L. Chen, Q. Kang, Q. Tang, B. A. Robinson, Y. He, and W. Tao, Pore-scale simulation of multicomponent multiphase reactive transport with dissolution and precipitation, Int. J. Heat Mass Transfer 85, 935 (2015).

[24] Y. Feng, M. Tayyab, and P. Boivin, A lattice-boltzmann model for low-mach reactive flows, Combust. Flame 196, 249 (2018).

[25] J. Kang, N. I. Prasianakis, and J. Mantzaras, Thermal multicomponent lattice boltzmann model for catalytic reactive flows, Phys. Rev. E 89, 063310 (2014).

[26] Y. Gan, A. Xu, G. Zhang, and S. Succi, Discrete boltzmann modeling of multiphase flows: hydrodynamic and thermodynamic non-equilibrium effects, Soft Matter 11, 5336 (2015).

[27] Y. Zhang, A. Xu, G. Zhang, Y. Gan, Z. Chen, and S. Succi, Entropy production in thermal phase separation: a kinetic-theory approach, Soft Matter 15, 2245 (2019).

[28] A. Xu, C. Lin, G. Zhang, and Y. Li, Multiple-relaxation-time lattice boltzmann kinetic model for combustion, Phys. Rev. E 91, 043306 (2015).

[29] C. Lin, A. Xu, G. Zhang, and Y. Li, Double-distribution-function discrete boltzmann model for combustion, Combust. Flame 164, 137 (2016).

[30] Y. Zhang, A. Xu, G. Zhang, C. Zhu, and C. Lin, Kinetic modeling of detonation and effects
of negative temperature coefficient, Combust. Flame 173, 483 (2016).

[31] C. Lin, K. H. Luo, L. Fei, and S. Succi, A multi-component discrete boltzmann model for nonequilibrium reactive flows, Sci. Rep. 7, 14580 (2017).

[32] C. Lin and K. H. Luo, Mesoscopic simulation of nonequilibrium detonation with discrete boltzmann method, Combust. Flame 198, 356 (2018).

[33] C. Lin, A. Xu, G. Zhang, Y. Li, and S. Succi, Polar-coordinate lattice boltzmann modeling of compressible flows, Phys. Rev. E 89, 013307 (2014).

[34] H. Lai, A. Xu, G. Zhang, Y. Gan, Y. Ying, and S. Succi, Nonequilibrium thermohydrodynamic effects on the rayleigh-taylor instability in compressible flows, Phys. Rev. E 94, 023106 (2016).

[35] C. Lin, A. Xu, G. Zhang, K. H. Luo, and Y. Li, Discrete boltzmann modeling of rayleigh-taylor instability in two-component compressible flows, Phys. Rev. E 96, 053305 (2017).

[36] F. Chen, A. Xu, and G. Zhang, Collaboration and competition between richtmyer-meshkov instability and rayleigh-taylor instability, Phys. Fluids 30, 102105 (2018).

[37] C. Lin and K. H. Luo, Mrt discrete boltzmann method for compressible exothermic reactive flows, Comput. Fluids 166, 176 (2018).

[38] C. Lin and K. H. Luo, Discrete boltzmann modeling of unsteady reactive flows with nonequilibrium effects, Phys. Rev. E 99, 012142 (2019).

[39] C. K. Batchelor, An introduction to fluid dynamics (Cambridge university press, Cambridge, 2000).

[40] M. K. Awasthi, R. Asthana, and G. Agrawal, Viscous correction for the viscous potential flow analysis of kelvin–helmholtz instability of cylindrical flow with heat and mass transfer, Int. J. Heat Mass Transfer 78, 251 (2014).

[41] G. Liu, Y. Wang, G. Zang, and H. Zhao, Viscous kelvin–helmholtz instability analysis of liquid–vapor two-phase stratified flow for condensation in horizontal tubes, Int. J. Heat Mass Transfer 84, 592 (2015).

[42] L. Wang, W. Ye, and Y. Li, Numerical investigation on the ablative kelvin-helmholtz instability, Europhys. Lett. 87, 54005 (2009).

[43] L. Wang, W. Ye, W. Don, Z. Sheng, Y. Li, and X. He, Formation of large-scale structures in ablative kelvin-helmholtz instability, Phys. Plasmas 17, 122308 (2010).

[44] Y. Gan, A. Xu, G. Zhang, C. Lin, H. Lai, and Z. Liu, Nonequilibrium and morphological characterizations of kelvin–helmholtz instability in compressible flows, Front. Phys. 14, 43602
(2019).

[45] C. Lin, K. H. Luo, Y. Gan, and Z. Liu, Kinetic simulation of nonequilibrium kelvin-helmholtz instability, Commun. Theor. Phys. **71**, 132 (2019).

[46] H. Zhang and F. Zhuang, Nnd schemes and their applications to numerical simulation of two- and three-dimensional flows, Adv. Appl. Mech. **29**, 193 (1991).

[47] R. B. Bird, Transport phenomena, Appl. Mech. Rev. **55**, R1 (2002).

[48] K. Qu, C. Shu, and Y. T. Chew, Alternative method to construct equilibrium distribution functions in lattice-boltzmann method simulation of inviscid compressible flows at high mach number, Phys. Rev. E **75**, 036706 (2007).

[49] Y. Gan, A. Xu, G. Zhang, Y. Zhang, and S. Succi, Discrete boltzmann trans-scale modeling of high-speed compressible flows, Phys. Rev. E **97**, 053312 (2018).

[50] Q. Li, Y. L. He, Y. Wang, and W. Q. Tao, Coupled double-distribution-function lattice boltzmann method for the compressible navier-stokes equations, Phys. Rev. E **76**, 056705 (2007).

[51] L. M. Yang, C. Shu, and Y. Wang, Development of a discrete gas-kinetic scheme for simulation of two-dimensional viscous incompressible and compressible flows, Phys. Rev. E **93**, 033311 (2016).

[52] Z. Guo, C. Zheng, and B. Shi, Non-equilibrium extrapolation method for velocity and pressure boundary conditions in the lattice boltzmann method, Chin. Phys. **11**, 366 (2002).

[53] M. Watari and M. Tsutahara, Two-dimensional thermal model of the finite-difference lattice boltzmann method with high spatial isotropy, Phys. Rev. E **67**, 036306 (2003).

[54] G. A. Sod, A survey of several finite difference methods for systems of nonlinear hyperbolic conservation laws, J. Comput. Phys. **27**, 1 (1978).

[55] W. C. Wan, G. Malamud, A. Shimony, C. A. Di Stefano, M. R. Trantham, S. R. Klein, D. Shvarts, C. C. Kuranz, and R. P. Drake, Observation of single-mode, kelvin-helmholtz instability in a supersonic flow, Phys. Rev. Lett. **115**, 145001 (2015).

[56] Y. Liu, P. Tan, and L. Xu, Kelvin-helmholtz instability in an ultrathin air film causes drop splashing on smooth surfaces, Proc. Natl. Acad. Sci. U.S.A. **112**, 3280 (2015).

[57] B. Akula, P. Suchandra, M. Mikhaeil, and D. Ranjan, Dynamics of unstably stratified free shear flows: an experimental investigation of coupled kelvin-helmholtz and rayleigh-taylor instability, J. Fluid Mech. **816**, 619 (2017).

[58] L. Wang, W. Ye, X. He, J. Wu, Z. Fan, C. Xue, H. Guo, W. Miao, Y. Yuan, J. Dong, G. Jia,
J. Zhang, Y. Li, J. Liu, M. Wang, Y. Ding, and W. Zhang, Theoretical and simulation research of hydrodynamic instabilities in inertial-confinement fusion implosions, Sci. China-Phys. Mech. Astron. 60, 055201 (2017).

[59] A. Xu, Finite-difference lattice-boltzmann methods for binary fluids, Phys. Rev. E 71, 066706 (2005).

[60] S. Arcidiacono, I. V. Karlin, J. Mantzaras, and C. E. Frouzakis, Lattice boltzmann model for the simulation of multicomponent mixtures, Phys. Rev. E 76, 046703 (2007).

[61] V. Sofonea and R. F. Sekerka, Bgk models for diffusion in isothermal binary fluid systems, Physica A 299, 494 (2001).

[62] S. A. Hosseini, N. Darabiha, and D. Thévenin, Mass-conserving advection-diffusion lattice boltzmann model for multi-species reacting flows, Physica A 499, 40 (2018).