Multiple-distribution-function lattice Boltzmann kinetic model for combustion phenomena

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A hybrid kinetic model for combustion phenomena is proposed. The chemical reaction process is described by a phenomenological rate function. The flow behavior is described by a Lattice Boltzmann Kinetic Model (LBKM) with any number of distribution functions. As an example, we illustrate the case with only two distribution functions. One distribution function is used to describe the reactant, and the other one is used to describe the reaction product. Compared with the traditional fluid model for combustion, the new model can be used to study simultaneously both the hydrodynamic and the thermodynamic nonequilibrium behaviors. Compared with the previous LBKM-hybrid models with single distribution function, the new model can be used to study more carefully the combustion process, for example, the variations of the particle number densities, particle mass densities, flow velocities, internal energies per unit volume, internal energies per unit mass, temperatures, and pressures of each species and the whole of the system. It is found that both of chemical reactant and reaction product have different levels of deviation from their equilibrium state in different degrees of freedom. For a special degree of freedom, the deviation of chemical reactant from its equilibrium state is different from that of reaction product from its equilibrium state.

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I. INTRODUCTION

More than 80% of world energy is created from combustion. The traditional numerical simulation of combustion is generally based on a hydrodynamic model combined with a phenomenological model for the chemical reaction process. The hydrodynamic model is generally the set of Euler equations or Navier-Stokes equations. The hydrodynamic model assumes that the system is nearly at its thermodynamic equilibrium and describes well the global fluid behavior of the system. But it has been known that the Thermodynamic NonEquilibrium (TNE) effects are pronounced in some cases, for example, around various interfaces. To describe simultaneously both the hydrodynamic and thermodynamic behaviors in the combustion procedure, a possible solution is to develop combustion models based on the Lattice Boltzmann Kinetic Model (LBKM).

There are two kinds of Lattice Boltzmann (LB) methods in literature. One kind is designed to solve various partial differential equations. The other kind aims to simulate the complex fluid behavior due to deviating from thermodynamic equilibrium. The latter is referred to LBKM. It is a special discretization of the Boltzmann equation. When the Knudsen number of the system is very small, the LBKM can be used to investigate both the hydrodynamic and thermodynamic behaviors.

Given the importance of combustion phenomena in daily life and engineering area, the LB simulating of combustion phenomena has been attempted from the early days of the LB studies. All those LB models mentioned above are for nearly incompressible systems which are valid only for combustion phenomena with very low Mach number, and they assume that the chemical reaction does not affect the flow fields. To model the more general case of combustion phenomena, LB model for compressible flows has to be developed.

Detonation is an important type of combustion, which travels through a shock wave with chemical reaction. It is widely used in various science and engineering areas, such as the acceleration of various projectiles, depositing of coating to a surface, cleaning of equipment, mining technologies, the research and analysis on coal and gas outburst mechanism, etc. Therefore, it is extensively studied in theory, experiment and numerical simulation. Since that the Mach number is larger than 1 is necessary for the existence of stable shock waves, the lattice Boltzmann model for detonation phenomena has to be applicable for supersonic flows. Several such lattice Boltzmann models have been proposed in recent
The first LBKM for detonation appeared in 2013. This model works for 2-dimensional system in Cartesian coordinates. A polar coordinate LBKM for detonation was given in 2014. Some very interesting nonequilibrium behaviors were presented. The two existing LBKMs for detonation use only one distribution function, which means there is only one set of hydrodynamic variables. The concentrations of the reactant and product are relevant to the parameter describing the chemical reaction process. Besides the detonation phenomena, the two models work also for combustion with Mach number less than 1. But via such models, we can not study the convection and thermal conduction, etc, between the reactant and product, let alone the thermodynamic nonequilibrium behaviors of various components. To make a more complete description of the combustion procedure, we resort to the LBKM hybrid model with multiple distribution functions. To this aim, we need firstly to choose a multiple-distribution-function kinetic model. In this side, in 2001 Sofonea and Sekerka proposed a nice Bhatnagar-Gross-Krook (BGK) model for isothermal binary fluid systems, where a split collision term model was discussed. In this work, we first extend the split collision term model to describe the thermal and high speed compressible fluid systems with any number of components. Then, combine it with a phenomenological reaction model to compose a multiple-distribution-function LBKM for combustion phenomena.

The rest of the paper is structured as follows. In section II we introduce the fluid system with multiple components. The new combustion model is constructed in section III. Section IV shows the validation and verification of the new model. Some interesting observations are presented in four cases. Section V summarizes and concludes the present paper.

II. FLUID SYSTEM WITH MULTIPLE COMPONENTS

We first consider a physical system composed of \( N \) kinds of fluid components, particles of component \( \sigma \) have mass \( m_\sigma \), where \( \sigma (= 1, 2, \cdots, N) \) is the index of the species of the components. The distribution function of component \( \sigma \) at the point \( (r, v) \) in phase space at time \( t \) reads \( f_\sigma \equiv f_\sigma(r, v, t) \). The particle number density, mass density and mean velocity of particles of species \( \sigma \) are

\[
\begin{align*}
n_\sigma &= \int f_\sigma dv, \\
\rho_\sigma &= m_\sigma n_\sigma,
\end{align*}
\]
\[ u_\sigma = \frac{1}{n_\sigma} \int f_\sigma d\mathbf{v}, \quad (3) \]

respectively. The particle number density, mass density and mean velocity of particles of physical system are

\[
\begin{align*}
n &= \sum_\sigma n_\sigma, \quad (4) \\
\rho &= \sum_\sigma \rho_\sigma, \quad (5) \\
u &= \frac{1}{\rho} \sum_\sigma \rho_\sigma u_\sigma, \quad (6)
\end{align*}
\]

respectively. The internal energy of species \( \sigma \) per unit volume and the one of physical system are

\[
\begin{align*}
E_\sigma &= m_\sigma \int \frac{1}{2} f_\sigma (\mathbf{v} - \mathbf{u})^2 d\mathbf{v}, \quad (7) \\
E &= \sum_\sigma E_\sigma, \quad (8)
\end{align*}
\]

respectively. The internal energy of species \( \sigma \) per unit mass and the one of physical system are

\[
\begin{align*}
e_\sigma &= E_\sigma / \rho_\sigma, \quad (9) \\
e &= E / \rho, \quad (10)
\end{align*}
\]

respectively. The energy equipartition theorem gives that

\[
\begin{align*}
E_\sigma &= n_\sigma \frac{D + I}{2} T_\sigma, \quad (11) \\
E &= n \frac{D + I}{2} T, \quad (12)
\end{align*}
\]

for thermodynamical system where each particle belonging to species \( \sigma \) has \( D + I \) degrees of freedom in a \( D \)-dimensional physical space. \( I \) is the number of extra degrees of freedom. Consequently, the temperature of species \( \sigma \) and that of the whole system are

\[
\begin{align*}
T_\sigma &= \frac{2E_\sigma}{n_\sigma(D + I)}, \quad (13) \\
T &= \frac{2E}{n(D + I)}, \quad (14)
\end{align*}
\]

respectively. The pressure of of species \( \sigma \) and that of physical system are

\[
\begin{align*}
P_\sigma &= n_\sigma T_\sigma, \quad (15)
\end{align*}
\]
\[ P = \sum_\sigma P_\sigma, \quad \text{(16)} \]

respectively. The adiabatic coefficient of the physical system is

\[ \gamma = \frac{D + I + 2}{D + I}. \quad \text{(17)} \]

In this work, we use the D2V33 discrete velocity model proposed by Watari\textsuperscript{23} for the physical system with \( D = 2, I = 0, \gamma = 2. \)

\section{III. HYBRID COMBUSTION MODEL}

\subsection{A. Model for chemical reaction}

Detonation is in a complex process. For simplicity, we use a phenomenological rate function to describe the process of chemical reaction. The Cochrans’s rate function\textsuperscript{24}

\[ \frac{d\lambda}{dt} = \omega_1 P^m (1 - \lambda) + \omega_2 P^n \lambda (1 - \lambda) \quad \text{(18)} \]

is a physically justifiable model which satisfies both simulation and experimental results in many cases\textsuperscript{25,26}. Here, the mass fraction of reacted reactant is

\[ \lambda = \frac{\rho_2}{\rho}, \quad \text{(19)} \]

where \( \rho_2 \) is the density of reacted reactant. The adjustable parameters are chosen as \( \omega_1 = 1, \omega_2 = 200, m = 1 \) and \( n = 1 \). The temporal derivative can be solved analytically\textsuperscript{19}, and the spatial derivatives can be calculated by adopting the nonoscillatory and nonfree-parameters dissipative finite difference scheme\textsuperscript{27}. Moreover, \( E > E_{ig} \) is a necessary condition for chemical reaction, with the ignition internal energy \( E_{ig} = 2.0. \)

With the release of chemical energy, the density \( \rho \) and velocity \( u \) of physical system remain unchanged, and other physical quantities changes in the following way,

\[ E^{\text{new}} = E + \rho q (\omega_1 P^m + \omega_2 P^n \lambda) (1 - \lambda) dt, \quad \text{(20)} \]

\[ \rho_1^{\text{new}} = \rho (1 - \lambda), \rho_2^{\text{new}} = \rho \lambda, \quad \text{(21)} \]

\[ n_1^{\text{new}} = \frac{\rho_1^{\text{new}}}{m_1}, n_2^{\text{new}} = \frac{\rho_2^{\text{new}}}{m_2}, n^{\text{new}} = n_1^{\text{new}} + n_2^{\text{new}}, \quad \text{(22)} \]

\[ T^{\text{new}} = \frac{2 E^{\text{new}}}{n^{\text{new}} (D + \varepsilon)}. \quad \text{(23)} \]
\[ P_{\text{new}} = n_{\text{new}} T_{\text{new}}, \]  

(24)

with \( q \) the amount of heat released by the chemical reactant per unit mass. It is clear from Eqs. (18) and (21) that \( \lambda \) changes from 0 to 1 in the progress of reaction, while \( \rho_1 \) reduces and \( \rho_2 \) increases with \( \rho_1 \geq 0 \) and \( \rho_2 \geq 0 \).

We consider a chemical reaction process where the reactant is composed of \( J \) species and the reaction product is composed of \( K \) species, as shown below,

\[ S_{11} + S_{12} + \cdots + S_{1J} \rightarrow S_{21} + S_{22} + \cdots + S_{2K}. \]  

(25)

If the mass concentration of each species of the reactants are well suitable for what required by the complete combustion, in other words, no reactant is remained after the complete reaction, the species number and the concentrations of the reaction products are determined by the chemical reaction itself. In this case, we have

\[ \rho_1 = \rho_{11} + \rho_{12} + \cdots + \rho_{1J}, \]  

(26)

\[ \rho_2 = \rho_{11} + \rho_{12} + \cdots + \rho_{1K}. \]  

(27)

Then, we can use Eqs. (19)-(24) to obtain the new hydrodynamic quantities after the chemical reaction but before the variation of the volume.

B. LBKM for flow behavior

The 2-dimensional system under consideration evolves according to the following LB equation\(^{23}\),

\[ \frac{\partial f_{\sigma,ki}}{\partial t} + v_{kix} \frac{\partial f_{\sigma,ki}}{\partial x} + v_{kiy} \frac{\partial f_{\sigma,ki}}{\partial y} = -\frac{1}{\tau_\sigma} (f_{\sigma,ki} - f^e_{\sigma,ki}), \]  

(28)

where \( f_{\sigma,ki} \) (\( f^e_{\sigma,ki} \)) is the discrete (equilibrium) distribution function of component \( \sigma \), \( \tau_\sigma \) is the relaxation time, and the discrete velocities \( v_{kix} = v_k \cos(i\pi/4) \) and \( v_{kiy} = v_k \sin(i\pi/4) \). The subscript \( k = 0, 1, 2, 3, 4 \) and \( i = 0, 1, \cdots, 7 \). In this work we choose \( v_0 = 0, v_1 = 1.5, v_2 = 3.5, v_3 = 7.5, v_4 = 12.5 \). The temporal and spatial derivatives of \( f_{\sigma,ki} \) in Eq. (28) can be solved in the same way as in Eq. (18).

The equilibrium distribution function is calculated in the following way,

\[ f^e_{\sigma,ki} = n_\sigma F_k \left[ (1 - \frac{u^2}{2\theta_\sigma}) + \frac{u^4}{8\theta^2_\sigma} \right] + \frac{v_{kix}u_x}{\theta_\sigma}(1 - \frac{u^2}{2\theta_\sigma}) + \frac{v_{kiy}u_y}{\theta^2_\sigma}(1 - \frac{u^2}{2\theta_\sigma}) \]

\[ + \frac{u_{kiu_i}}{6\theta^3_\sigma} + \frac{v_{kiu_i}v_{kiu_j}u_iu_ju_\theta}{24\theta^4_\sigma} \]  

(29)
with coefficients

\[ F_k = \frac{1}{v_k^2(v_k^2 - v_{k+1}^2)(v_k^2 - v_{k+2}^2)} \left[ 48\theta^4 - 6(v_{k+1}^2 + v_{k+2}^2 + v_{k+3}^2)\theta^3 + (v_{k+1}^2 v_{k+2}^2 + v_{k+2}^2 v_{k+3}^2 + v_{k+3}^2 v_{k+1}^2)\theta^2 + \frac{1}{4}v_{k+1}^2 v_{k+2}^2 v_{k+3}^2 \theta \right] \]

\[ F_0 = 1 - 8(F_1 + F_2 + F_3 + F_4), \]

\[ \theta = T/m_\sigma, \]

where the subscript \( \{k + l\} \) equals \( (k + l - 4) \) if \( (k + l) > 4 \).

The LBKM has the ability to investigate the nonequilibrium behaviors of the physical system by using the high-order moments of \( f_{\sigma,ki} \) and \( f_{\sigma,ki}^{eq} \). The manifestations of nonequilibrium are\(^{12,20} \)

\[ \begin{align*}
\Delta^*_2(\sigma) &= \sum_{ki}(f_{\sigma,ki} - f_{\sigma,ki}^{eq})v^*_{ki}v^*_{ki} \\
\Delta^*_3(\sigma) &= \sum_{ki}(f_{\sigma,ki} - f_{\sigma,ki}^{eq})v^*_{ki}v^*_{ki}v^*_{ki} \\
\Delta^*_3,1(\sigma) &= \sum_{ki} \frac{1}{2}(f_{\sigma,ki} - f_{\sigma,ki}^{eq})v^*_{ki} \cdot v^*_{ki}v^*_{ki} \\
\Delta^*_4,2(\sigma) &= \sum_{ki} \frac{1}{2}(f_{\sigma,ki} - f_{\sigma,ki}^{eq})v^*_{ki} \cdot v^*_{ki}v^*_{ki}v^*_{ki}
\end{align*} \] (30)

with \( v^*_{ki} = v_{ki} - u \).

IV. NUMERICAL SIMULATIONS

As an example, we illustrate only the case where all the reactant components are globally described by only one distribution function, \( f_1 \), and all the product components are globally described by only one distribution function, \( f_2 \). In this section, we numerical study four cases: (i) \( q = 0, m_1 = m_2 = 1 \), (ii) \( q = 0, m_1 = 1, m_2 = 2 \), (iii) \( q = 0, m_1 = 2, m_2 = 1 \), (iv) \( q = 1.2, m_1 = 2, m_2 = 1 \). The initial conditions for each case satisfy the Hugoniot relations for detonation wave. In the first three cases no reaction heat is released. Intuitively, the hydrodynamic quantities of the whole system in case (i) show the same behaviors as in the pure shocking process. In case (ii) or (iii), even though the mass density, flow velocity, internal energy per unit volume, internal energy per unit mass and pressure of the whole system show the same behaviors as in the pure shocking process, the particle number density and temperature of the whole system show different behaviors from those in the pure shocking process. Case (iv) shows a real detonation process.
FIG. 1. physical quantities in the case of \( q = 0, \ m_1 = 1, \ m_2 = 1 \) at time \( t = 0.25 \): (a) particle number density, (b) particle mass density, (c) velocity, (d) internal energy per unit volume, (e) internal energy per unit mass, (f) temperature, (g) pressure, (h) \( \lambda \).

A. **Case of \( q = 0, \ m_1 = 1 \) and \( m_2 = 1 \)**

The initial physical quantities read

\[
\begin{aligned}
(\rho, T, u_x, u_y, \lambda)_L &= (2.19087, 3.14356, 1.78885, 0, 1) \\
(\rho, T, u_x, u_y, \lambda)_R &= (1, 1, 0, 0, 0)
\end{aligned}
\]

(31)

where the suffix \( L \) indexes the left part \((0,0.1)\) and \( R \) the right part \((0.1,1)\). The quantities at the two parts satisfy Hugoniot relations for shock wave. Other parameters are \( \tau_1 = \tau_2 = 10^{-7} \), \( N_x \times N_y = 1000 \times 1 \), \( dx = dy = 0.001 \), \( dt = 5 \times 10^{-7} \). The symbol \( \sigma = 1 \) indicates the chemical reactant, and \( \sigma = 2 \) its product.

Figure\( \Box \) shows physical quantities in the case of \( q = 0, \ m_1 = 1, \ m_2 = 1 \) at time \( t = 0.25 \). Each of panels (a)-(g) gives quantities of the whole physical system, the chemical reactant and the reaction product. Panel (h) gives the mass fraction of reacted reactant. The reaction area is where \( \lambda \) changes from 0 to 1. Figure\( \Box \) successfully recovers the following fundamental relations. (i) The quantities \( (n_2, \rho_2, u_{x2}, E_2, e_2, T_2, P_2) \) of the product equal zero in front of the reaction area, and the quantities \( (n_1, \rho_1, u_{x1}, E_1, e_1, T_1, P_1) \) of the reactant are zero
FIG. 2. physical quantities in the case of $q = 0, m_1 = 1, m_2 = 2$ at time $t = 0.25$: (a) particle number density, (b) particle mass density, (c) velocity, (d) internal energy per unit volume, (e) internal energy per unit mass, (f) temperature, (g) pressure, (h) $\lambda$.

behind the reaction area. (ii) $n = n_1 + n_2$, $\rho = \rho_1 + \rho_2$, $E = E_1 + E_2$, $P = P_1 + P_2$, $u_x = u_{x1} = u_{x2}$, $T = T_1 = T_2$ in the whole physical area. Numerically, $\rho = 2.19042$, $u_x = 1.78828$, $P = 6.89025$ behind the reaction area, and the relative deviations of the three quantities from the theoretical results given by Eq.31 are about 0.02%, 0.03%, 0.04%, respectively. That’s to say, the simulation results have a satisfying agreement with the theoretical ones.

B. Case of $q = 0$, $m_1 = 1$ and $m_2 = 2$

The initial physical quantities and other parameters are the same as the above case.

Similar to Fig.1 Fig.2 shows physical quantities in the case of $q = 0, m_1 = 1, m_2 = 2$ at time $t = 0.25$. The simulation results give $\rho = 2.19044$, $u_x = 1.78831$, $P = 6.89008$ behind reaction area in Fig.2. The deviations of them from the theoretical results are about 0.02%, 0.03%, 0.04%, respectively. Consequently, the simulation results have a satisfying agreement with the theoretical ones.
FIG. 3. Physical quantities in the case of $q = 0$, $m_1 = 2$, $m_2 = 1$ at time $t = 0.25$: (a) particle number density, (b) particle mass density, (c) velocity, (d) internal energy per unit volume, (e) internal energy per unit mass, (f) temperature, (g) pressure, (h) $\lambda$.

A more careful analysis of Fig. 2 is referred to the next subsection.

C. Case of $q = 0$, $m_1 = 2$ and $m_2 = 1$

The initial physical quantities and other parameters are the same as in the first case.

Figure 3 shows physical quantities in the case of $q = 0$, $m_1 = 2$, $m_2 = 1$ at time $t = 0.25$. Numerically, $\rho = 2.19036$, $u_x = 1.78821$, $P = 6.89063$ behind the reaction area. Their relative deviations from the theoretical results are about 0.02%, 0.04%, 0.05%, respectively. Also, the simulation results have a satisfying agreement with the theoretical ones.

It is easy to find that $\rho$, $\rho_1$, $\rho_2$, $u_x$, $u_{x1}$, $u_{x2}$, $E$ and $\lambda$ in Fig. 3 show the same behaviors as those in Fig. 1 or 2. Physically, what satisfy the Hugoniot relations for the detonation/shock wave are the particle mass density, the flow velocity and the internal energy of the whole physical system. The three physical quantities are not under the influence of any kind of particle mass in the detonation process. Consequently, $\rho$, $u_x$ and $E$ in Fig. 3 are the same as the ones in Fig. 1 or 2. Equation 18 shows that $\lambda$ is not affected by the particle masses, so it
is the same in the three figures. Hence, $\rho_1$ and $\rho_2$ in Fig. 3 are the same as the ones in Fig. 1 or 2. Because $u_{x1} = u_{x2} = u$, $u_{x1}$ and $u_{x2}$ in the three figures show the same behaviors.

More attention should be paid to the particle number densities, the internal energies per unit mass and the temperatures in Figs. 1-3. Firstly, the results of $n_1$ in Fig. 1 and Fig. 3 are the same due to $m_1 = 1$ in the two figures; the results of $n_2$ in Fig. 1 and Fig. 3 are the same due to $m_2 = 1$ in the two figures; $n_1$ in Fig. 3 is quite different from that in Fig. 1 or 2. $n_2$ in Fig. 2 is quite different from that in Fig. 1 or 3. Consequently, the results of $n$ in the Figs. 1-3 are different. Secondly, Fig. 2 gives that $n$ shows a peak at the point $x = 0.9205$ where the growth rate of $T$ reduces; Fig. 3 gives that $T$ shows a peak at the point $x = 0.9205$ where the growth rate of $n$ reduces. Mathematically, Eq. 14 gives that $T$ is a function of $n$ for a given specific case of $E$. Thirdly, $e_1 < e < e_2$ in Fig. 3 due to $m_1 > m_2$, $e_1 = e = e_2$ in Fig. 1 due to $m_1 = m_2$, $e_1 > e > e_2$ in Fig. 2 due to $m_1 < m_2$. Mathematically, Eqs. 2, 3 and 9-12 give that $e_\sigma = [(D + I)T]/(2m_\sigma)$, i.e., $e_\sigma$ is a function of $m_\sigma$ for a given specific case of $T$, and $e$ is a weighted average of $e_\sigma$.

Figure 4 shows the simulation results of $\Delta^\star(\sigma)$ in the same case as in Fig. 3. The first row
is for fluid component $\sigma = 1$, and the second for $\sigma = 2$. Only independent components of $\Delta_2^*(\sigma), \Delta_3^*(\sigma), \Delta_{3,1}^*(\sigma), \Delta_{4,2}^*(\sigma)$ are shown in each panel. The specific correspondences are referred to the legends. A vertical dashed line is shown in each panel to guide the eye for the position $x = 0.9185$. Firstly, $\Delta_{2,xy}^*(\sigma), \Delta_{3,xx}^*(\sigma), \Delta_{3,yy}^*(\sigma), \Delta_{3,1,y}^*(\sigma), \Delta_{4,2,xy}^*(\sigma)$ equal zero due to the symmetry of the physical system in the $y$ direction. Secondly, the results of $\Delta^*(1)$ and $\Delta^*(2)$ are quite different along $x$ axis. Thirdly, panels (a) and (e) show that $\Delta_{2,xx}^*(1) > 0$, $\Delta_{2,yy}^*(1) < 0$, $\Delta_{2,xx}^*(2) > 0$, $\Delta_{2,yy}^*(2) < 0$ on the right side of the vertical dashed line, $\Delta_{2,xx}^*(1) > 0$, $\Delta_{2,yy}^*(1) > 0$, $\Delta_{2,xx}^*(2) < 0$, $\Delta_{2,yy}^*(2) < 0$ on the left side, and $\Delta_{2,xx}^*(1) + \Delta_{2,yy}^*(1) \neq 0$, $\Delta_{2,xx}^*(2) + \Delta_{2,yy}^*(2) \neq 0$ across the reaction area. Fourthly, panels (b), (c), (f) and (g) show that $\Delta_{3,xxx}^*(1), \Delta_{3,xyy}^*(1)$ and $\Delta_{3,1,x}^*(1)$ have a crest and trough across the reaction area where $\Delta_{3,xxx}^*(2), \Delta_{3,xyy}^*(2)$ and $\Delta_{3,1,x}^*(2)$ have only a crest across the reaction area, and $\Delta_{3,xxx}^*(\sigma) + \Delta_{3,xyy}^*(\sigma) = 2\Delta_{3,1,x}^*(\sigma), \Delta_{3,xyy}^*(\sigma) + \Delta_{3,yyy}^*(\sigma) = 2\Delta_{3,1,y}^*(\sigma)$. Finally, troughs of $\Delta_{3,xxx}^*(1), \Delta_{3,xyy}^*(1), \Delta_{3,1,x}^*(1)$ and the peaks of $\Delta_{3,xxx}^*(2), \Delta_{3,xyy}^*(2), \Delta_{3,1,x}^*(2)$ are almost at the same point.

D. Case of $q = 1.2$, $m_1 = 2$ and $m_2 = 1$

The above three numerical tests are for the cases with chemical reaction but without released reaction heat, which are not the real combustion procedures. In this subsection we study the case with $q > 0$. As an example, we first choose $q = 1.2$. The comparison with the case in subsection C gives indication for the effects of the size of $q$. The initial physical quantities read

$$
\begin{cases}
(\rho, T, u_x, u_y, \lambda)_L = (1.37321, 2.87178, 0.894427, 0, 1) \\
(\rho, T, u_x, u_y, \lambda)_R = (1, 1, 0, 0, 0)
\end{cases}
$$

(32)

The quantities in Eq.32 satisfy Hugoniot relations for detonation wave.

Figure 5 shows physical quantities in the case of $q = 1.2$, $m_1 = 2$, $m_2 = 1$ at time $t = 0.25$. The simulation results $\rho = 1.37866$, $u_x = 0.896802$, $P = 3.90949$ behind the reaction area. The deviations of them from the theoretical results in Eq.32 are about 0.40%, 0.26%, 0.86%, respectively. That’s to say, the simulation results have a satisfying agreement with the theoretical ones. First, all quantities of the whole system, the reactant and the reaction product show peaks across the detonation wave in the reaction area. Second, panels (a), (b), (d), (e), (g) show that, with the detonation wave travelling forwards, $n_1$, $\rho_1$, $E_1$, ...
FIG. 5. physical quantities in the case of $q = 1.2$, $m_1 = 2$, $m_2 = 1$ at time $t = 0.25$: (a) particle number density, (b) particle mass density, (c) velocity, (d) internal energy per unit volume, (e) internal energy per unit mass, (f) temperature, (g) pressure, (h) $\lambda$.

$e_1$, $P_1$ first reach their peaks, then $n$, $\rho$, $E$, $e$, $P$ get their maximums, and last $n_2$, $\rho_2$, $E_2$, $e_2$, $P_2$. Third, $u = u_{x_1} = u_{x_2}$, $T = T_1 = T_2$ across the detonation wave, and they get their maximums almost at the same time.

There are two main differences between Figs. 3 and 5. On the one hand, $n_2$, $\rho_2$, $E_2$, $P_2$ in Fig. 5 increase and then reduce across the detonation wave, while the ones in Fig. 3 always increase. On the other hand, Fig. 3 gives that the growth rate of $n$ reduces around $x = 0.9205$, where $T$ reaches its maximum, while Fig. 5 gives that both of $n$ and $T$ show peaks. Obviously, the differences result from the released chemical energy.

Similar to Fig. 4, Fig. 6 shows the simulation results of $\Delta^*(\sigma)$ in the case of $q = 0$, $m_1 = 2$, $m_2 = 1$ at time $t = 0.25$. A vertical dashed line is shown in each panel to guide the eye for the position $x = 0.8895$.

It is found that the simulation results of $\Delta^*(\sigma)$ in Fig. 4 are similar to the ones in Fig. 6 on the right sides of the vertical dashed lines, and $\Delta_{3,1}^*(1)$, $\Delta_{3,1}^*(1)$ and $\Delta_{4,2}^*(1)$ in Fig. 4 are similar to the ones in Fig. 6 in the whole area. The differences between the two figures are as: (i) the result of $\Delta^*_{2,xx}(1)$ on the left side of the line in Fig. 4 (a) is greater than zero,
FIG. 6. The non-equilibrium manifestations $\Delta^*_m$ in the case of $q = 1,2$, $m_1 = 2$, $m_2 = 1$ at time $t = 0.25$. Panels (a)-(h) are for $\Delta^*_2(1)$, $\Delta^*_3(1)$, $\Delta^*_3,1(1)$, $\Delta^*_4,2(1)$, $\Delta^*_5(2)$, $\Delta^*_5,1(2)$, $\Delta^*_4,2(2)$, respectively. Only independent components of $\Delta^*(\sigma)$ are shown.

while the one in Fig. (a) is only a little less than zero. (ii) $\Delta^*_{2,yy}(2) < 0$ on the left side in Fig. (e), while $\Delta^*_{2,yy}(2) > 0$ on the left side of line in Fig. (e). (iii) Each of $\Delta^*_{3,xxx}(2)$, $\Delta^*_{3,xyy}(2)$, $\Delta^*_{3,1,x}(2)$ in Fig. (f) shows only a peak, while each of them in Fig. (f) shows a trough and crest. (iv) $\Delta^*_{4,2,yy}(2)$ is close to zero on the left side in Fig. (h), while $\Delta^*_{4,2,yy}(2)$ is greater than zero on the left side in Fig. (h). The above differences result from the released chemical energy which accelerates the detonation wave. Both the reactant and its product are compressed in front of the von-Neumann-peak due to the pre-shocking process, while they are under rarefaction effect behind the peak with chemical energy being released.

V. CONCLUSIONS

A hybrid kinetic model for combustion phenomena is proposed. The chemical reaction process is described by a phenomenological rate function. The flow behavior is described by a Lattice Boltzmann Kinetic Model (LBKM) with any number of distribution functions. Compared with the traditional fluid model for combustion, the new model can be used
to study simultaneously both the hydrodynamic and the thermodynamic nonequilibrium behaviors. Compared with the previous hybrid models with single distribution function, the new model can be used to study more details of the combustion process, for example, the variations of the particle number densities, particle mass densities, flow velocities, internal energies per unit volume, internal energies per unit mass, temperatures, and pressures of each species and the whole of the system.

In fact, chemical reactant and reaction product may be composed of various components. Given proportions of mass densities of the components belonging to the chemical reactant and reaction product, and given the particle masses, we can get all the above-mentioned physical quantities from the LB evolution of the discrete distribution function of each component. In this work, for simplicity, we illustrate the case where all the reactant components are globally described by only one distribution function, $f_1$, and all the product components are globally described by only one distribution function, $f_2$.

The particle number densities of the whole physical system and the chemical reactant show peaks around the detonation wave when the particle mass of reactant is less than that of reaction product in the case of released chemical energy approaching zero. The temperatures of the whole physical system, the reactant and the reaction product show peaks around the detonation wave when the particle mass of reactant is greater than that of reaction product in the same case.

Some interesting nonequilibrium behaviors are presented. For example, both of chemical reactant and reaction product have different levels of deviation from their equilibrium state in different degrees of freedom. For a special degree of freedom, the deviation of chemical reactant from its equilibrium state is different from that of reaction product from its equilibrium state. For either chemical reactant or reaction product, “the energy flow caused by microscopic fluctuation” in the propagative direction of the detonation wave approaches extremum at about the von Neumann peak.

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