Multiple-relaxation-time lattice Boltzmann kinetic model for combustion

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Abstract

To probe both the Mechanical Non-Equilibrium (MNE) and Thermodynamic Non-Equilibrium (TNE) in the combustion procedure, a two-dimensional Multiple-Relaxation-Time (MRT) version of the Lattice Boltzmann Kinetic Model (LBKM) for combustion phenomena is presented. The chemical energy released in the progress of combustion is dynamically coupled into the system by adding a chemical term to the LB kinetic equation. The LB model is required to recover the Navier-Stokes equations with chemical reaction in the hydrodynamic limit. To that aim, we construct a discrete velocity model with 24 velocities divided into 3 groups. In each group a flexible parameter is used to control the size of discrete velocities and a second parameter is used to describe the contribution of the extra degrees of freedom. The current model works for both subsonic and supersonic flows with or without chemical reaction. In this model both the specific-heat ratio and the Prandtl number are flexible, the TNE effects are naturally presented in each simulation step. Via the MRT model, it is more convenient to track the effects of TNE and how the TNE influence the MNE behaviors. The model is verified and validated via well-known benchmark tests. It is found that around the detonation wave there are competition between the viscous effect, thermal diffusion effect and the gradient effects of physical quantities. Consequently, with decreasing the collision parameters, (i) the nonequilibrium region becomes wider and the gradients of physical quantities decrease; (ii) the position where the internal energy in the shocking degree of freedom equals the one averaged over all degrees of freedom moves away from the position for the von Neumann peak.

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I. INTRODUCTION

The combustion has long been playing a dominant role in the transportation and power generation. More than 80% of world energy is from various combustion processes. For a foreseeable future it will remain to be the major energy conversion process \[1\]. At the same time, the low energy conversion efficiency of existing combustion engines has been becoming the major source of air pollution and driving force for climate change \[2\]. Roughly speaking, there are two kinds of fuels, the nuclear fuel and the organic fuel. The latter contains the organic materials such as hydrocarbon natural fuel and artificial fuel after processing. Various medical wastes \[3\] belong to the organic fuel. To achieve low emissions, fuel lean and high speed combustion and enable new engine technologies, in recent years, some new combustion concepts, such as pulsed and spinning detonation engines \[4, 5\], microscale combustion \[6, 7\] and nanopropellants \[8, 9\], partially premixed and stratified combustion \[10\], plasma assisted combustion \[11, 13\], and cool flames \[14\], have been proposed and developed.

However, there are still a number of problems, for example, (i) for spinning detonation, the influences of the wall curvature and fuel/air mixing on the detonation initiation and propagation modes, (ii) for high pressure stratified combustion, the ignition to detonation transition at low temperature, (iii) for plasma assisted combustion, the highly non-equilibrium energy transfer between electrons, electronically and vibrationally excited molecules, and neutral molecules, (iv) for cool flames, the hydrodynamics, chemical kinetics, and kinetics-transport coupling, are challenging our current understanding \[1, 15–17\]. All these new combustion concepts involve complicated non-equilibrium chemical and transport processes.

For a long time, the main way people know the combustion process is experimental and theoretical research \[18–24\]. In recent five decades, the numerical simulation of combustion process has achieved great success \[24–28\]. To simulate a combustion procedure, the following steps are needed. (i) Establish a physical model. (ii) Establish discrete control equations. (iii) Numerical experiments and data analysis. Generally speaking, for a combustion system, there are three levels of description which are in the microscopic, mesoscopic and macroscopic scales, respectively. The microscopic scale is generally referred to the description at Molecular Dynamic (MD) level. The main numerical tool is the MD simulation. Via study at this level, the reaction rate equation can be established. The macroscopic scale
is generally referred to the description based on Navier-Stokes equations. At this level the mainly concerned are Mechanical Non-Equilibrium (MNE) effects, specifically, the behaviors of the density, temperature, flow velocity and pressure. The mesoscopic description is generally referred to the description based on the gas kinetic theory, more specifically, the Boltzmann equation. At this level, we can study more details of the interfacial structures and Thermodynamic Non-Equilibrium (TNE) effects.

What used in the most engineering applications is the macroscopic description or hydrodynamic description. The physical model at this level consists of some specific form of the hydrodynamic equations coupled with some phenomenological reaction rate equation, which is constructed according to the conservation laws of mass, momentum and energy, as well as some suitable simplifications. To establish the discrete control equations, the first step is to choose a coordinate system where the coordinate axes should adapt to the edge of the computational/physical domain. When the computational domain is rectangle, cylindrical or conical, the generally chosen coordinate system can be orthogonal, cylindrical, or spherical. The second step is to establish a structured, unstructured or block-structured grid according to the specific situation. The third step is to choose or formulate a discretization scheme. The frequently used schemes includes the Finite Difference (FD), the finite volume, the finite element, the finite analysis, the boundary element, the integration transformation, the spectral method, etc.

In recent nearly three decades the Lattice Boltzmann (LB) method [29–48] has been becoming a powerful tool to simulate various complex flows. Due the importance of combustion phenomena and the quick development of LB method, one can find a number of papers in literature [49–66]. The pioneering LB model for combustion systems was given by Succi et al. [49] in 1997. This work is based on the assumptions of fast chemistry and cold flames with weak heat release. In the following years, Filippova and Hänel [50–52] proposed and developed a kind of hybrid scheme for low Mach number reactive flows. The flow field is solved by modified lattice-BGK method and the transport equations for energy and species are solved by a FD scheme. Via the LB method Yu et al. [53] simulated scalar mixing in a multi-component flow and a chemical reacting flow. Yamamoto et al. [54] proposed a LB method for combustion phenomena including the reaction, diffusion and convection effects. Lee et al. presented a Double-Distribution Function LB model to solve the laminar diffusion flames within the context of Burke-Schumann flame sheet model. In recent years Chen et al
developed a coupled LB method for the low Mach number combustion and presented some meaningful results.

In brief, LB modeling of combustion phenomena has long been an interesting topic, but was mainly focused on low Mach number combustion where the incompressible LB model works. In those studies the LB model works as a kind of new scheme to recover the hydrodynamic model. In those thermal LB models, the temperature $T$ could not be described by the same Distribution Function (DF) which describes the density $\rho$ and flow velocity $u$. In some LB models it was further assumed that the chemical reaction has no effect on the flow field.

As a special case of combustion, the explosion phenomena lead to accidents or disasters sometimes. But the controlled explosion has been widely applied in various engineering problems, such as, explosion painting, explosion cleaning, explosion working, explosion propulsion, demolition blasting, blasting mining, blasting excavation, etc. The traditional computational fluid dynamics has been used to simulate explosion for many years. It is interesting to extend the LB model to simulate such complex phenomena. As a special discretization of the Boltzmann equation, the appropriately designed LB model should possess more kinetic information which is beyond the description of the Navier-Stokes equations.

To model a more practical combustion phenomenon, an appropriate LB Kinetic Model (LBKM) should be thermal, compressible, and work for both the low and the high Mach number flows. At the same time, the chemical reaction and flow behavior should couple naturally. In such a LB kinetic model, the density $\rho$, flow velocity $u$, temperature $T$ and relevant higher-order moments should be described by the same DF. It should work as a new tool to probe both the MNE and TNE.

In recent years the development of LB models for high speed compressible flows makes it possible to simulate systems with shock wave. Very recently we presented two LB models for high Mach combustion and detonation phenomena. The first is in Cartesian coordinates. The second is in polar coordinate system, which is more convenient for simulating the explosion and implosion behaviors. Both the two models are based on the Single-Relaxation-Time (SRT) BGK-Boltzmann equation. Consequently, the Prandtl number is fixed at 1. A solution to this problem is to use a Multiple-Relaxation-Time (MRT) version of the LB model. Early in 1989, Higuera, Succi and Benzi developed an efficient strategy for building suitable collision operators, which is used in a simplified version.
of the lattice gas Boltzmann equation \[29\]. This work is the precursor of all MTR models \[30, \[31, \[73, \[74, \[79\], etc. In this work we present a MRT kinetic LB model for low and high Mach number combustion phenomena. In the new model, since the collision term is first calculated in the moment space and then transformed back to the discrete velocity space, not only the viscosity and heat conductivity can be adjusted independently, but also the behaviors due to deviating from thermodynamic equilibrium are naturally obtained/calculated in each simulation step. Physically, it is more convenient to follow how the TNE behave and influence the system evolution.

The rest of the paper is organized as below. In section II the MRT version of LBKM for combustion is formulated. In section III we demonstrate that the new model can recover the Navier-Stokes equations with chemical reaction in the hydrodynamic limit. The validation and verification of the MRT-LBKM are presented in section IV. Some results on detailed structures of the detonation wave are shown in Section V. Section VI summarizes and concludes the present paper.

II. FORMULATION OF THE LATTICE BOLTZMANN KINETIC MODEL

The practical combustion process is very complicated. To study some fundamental behaviors in the combustion system, in this work we propose a simple LBKM described by the following equation,

\[
\frac{\partial f_i}{\partial t} + v_{i\alpha} \frac{\partial f_i}{\partial r_{\alpha}} = -M_{il}^{-1} \left[ \hat{R}_{lk} \left( \hat{f}_k - \hat{f}_k^{eq} \right) + \hat{A}_l \right] + C_i, \tag{1}
\]

\[
C_i = \left. \frac{df_i}{dt} \right|_{R(\lambda)} \tag{2}
\]

where \(i = 1,2,\ldots,N\) is the index of discrete velocity, \(N\) is the total number of the discrete velocity used in the LBKM, \(f_i\) is the discrete distribution function, \(v_{i\alpha}\) is the \(\alpha\)-component of the \(i\)-th discrete velocity, \(\alpha = x, y\); \(\hat{f}_k = M_{ki} f_i \ (\hat{f}_k^{eq} = M_{ki} f_i^{eq})\) is the moment of the (equilibrium) distribution function and formally the (equilibrium) distribution function in the moment space; \(M_{ki}\) is the element of the matrix \(\mathbf{M}\) connecting the vector of discrete distribution function, \(\mathbf{f} = (f_1, f_2, \ldots, f_N)^T\), and the vector, \(\hat{\mathbf{f}} = (\hat{f}_1, \hat{f}_2, \ldots, \hat{f}_N)^T\); \(\hat{\mathbf{R}} = \mathbf{MM}^{-1} = \text{diag}(R_1, R_2, \ldots, R_N)\) is a diagonal matrix whose element \(R_k\) describes speed of \(\hat{f}_k\) approaching \(\hat{f}_k^{eq}\); \(\hat{A}_l\) is the \(l\)-th element of \(\hat{\mathbf{A}} = (0, \ldots, 0, \hat{A}_8, \hat{A}_9, 0, \ldots, 0)^T\) and is a
modification to the collision operator \( \hat{R}_{lk} (\hat{f}_k - \hat{f}_k^{eq}) \), where

\[
\hat{A}_8 = \rho T \frac{R_5 - R_8}{R_5} \left[ 4u_x \left( \frac{\partial u_x}{\partial x} - \frac{1}{D + I} \frac{\partial u_y}{\partial x} - \frac{1}{D + I} \frac{\partial u_y}{\partial y} \right) + 2u_y \left( \frac{\partial u_y}{\partial x} + \frac{\partial u_x}{\partial y} \right) \right],
\]

\[
\hat{A}_9 = \rho T \frac{R_7 - R_9}{R_7} \left[ 4u_y \left( \frac{\partial u_x}{\partial y} - \frac{1}{D + I} \frac{\partial u_x}{\partial x} - \frac{1}{D + I} \frac{\partial u_y}{\partial y} \right) + 2u_x \left( \frac{\partial u_y}{\partial x} + \frac{\partial u_x}{\partial y} \right) \right].
\]

The reason for this modification is as below. Although from the mathematical point of view, the relaxation coefficient \( R_k \) can be independently adjusted for each kinetic mode \( (\hat{f}_k - \hat{f}_k^{eq}) \), from the physical point of view, coupling may exist between or among different kinetic modes. The Chapman-Enskog analysis helps to find back the missing coupling.\[74\]

This modification is added so that the LBKM can recover the consistent Navier-Stokes equations in the hydrodynamic limit. \( C_i \) is the chemical term added to the LB equation and will be given a specific form in the following part. For convenience of description below, we introduce \( A_i = M_i^{-1} \hat{A}_i \). In this work we consider a two-dimensional \( (D = 2) \) system where the particle mass is unity. The discrete equilibrium distribution function satisfies the following relations

\[
\sum f_i^{eq} = \rho = \sum f_i,
\]

\[
\sum f_i^{eq} v_{i\alpha} = \rho u_\alpha = \sum f_i v_{i\alpha},
\]

\[
\sum f_i^{eq} (v_i^2 + \eta_i^2) = \rho [(D + I)T + u^2] = \sum f_i (v_i^2 + \eta_i^2),
\]

\[
\sum f_i^{eq} v_{i\alpha} v_{i\beta} = \rho (\delta_{\alpha\beta} T + u_\alpha u_\beta),
\]

\[
\sum f_i^{eq} (v_i^2 + \eta_i^2) v_{i\alpha} = \rho u_\alpha [(D + I + 2)T + u^2],
\]

\[
\sum f_i^{eq} v_{i\alpha} v_{i\beta} v_{i\chi} = \rho (u_\alpha \delta_{\beta\chi} + u_\beta \delta_{\chi\alpha} + u_\chi \delta_{\alpha\beta}) T + \rho u_\alpha u_\beta u_\chi,
\]

\[
\sum f_i^{eq} (v_i^2 + \eta_i^2) v_{i\alpha} v_{i\beta} = \rho \delta_{\alpha\beta} [(D + I + 2)T + u^2] + \rho u_\alpha u_\beta [(D + I + 4)T + u^2],
\]

\[
\sum f_i^{eq} \eta_i^2 v_{i\alpha} v_{i\beta} = \rho \delta_{\alpha\beta} IT^2 + \rho u_\alpha u_\beta IT,
\]

\[
\sum f_i^{eq} (v_i^2 + \eta_i^2) \eta_i^2 = \rho IT [u^2 + (D + 3)T],
\]

\[
\sum f_i^{eq} (v_i^2 + \eta_i^2) v_{i\alpha} = \rho u_\alpha [u^4 + (D + 2)(D + I + 4)T^2 + (2D + I + 8)u^2 T],
\]

\[
\sum f_i^{eq} (v_i^2 + \eta_i^2) \eta_i^2 v_{i\alpha} = \rho u_\alpha IT [u^2 + (D + 3I + 2)T],
\]

where \( \rho, T, p (= \rho T) \), and \( u_\alpha \) are the density, temperature, pressure and velocity, respectively.

Besides the translational degrees of freedom, \( \eta_i \) is a free parameter introduced to describe the
I extra degrees of freedom corresponding to molecular rotation and/or internal vibration. The internal kinetic energy per unit volume is \( E = \rho(D + I)T/2 \).

Actually, Eqs. (5)-(15) can be uniformly written in a matrix form, i.e.,

\[
\mathbf{M} \times \mathbf{f}^{eq} = \hat{\mathbf{f}}^{eq},
\]

where the bold-face symbols, \( \mathbf{f}^{eq} = (f_{1}^{eq}, f_{2}^{eq}, \ldots, f_{N}^{eq})^T \) and \( \hat{\mathbf{f}}^{eq} = (\hat{f}_{1}^{eq}, \hat{f}_{2}^{eq}, \ldots, \hat{f}_{N}^{eq})^T \), denote N-dimensional column vectors. The matrix \( \mathbf{M} = (M_{1}, M_{2}, \ldots, M_{N})^T \), \( M_{i} = (m_{i1}, m_{i2}, \ldots, m_{iN}) \), where \( m_{i1} = 1, m_{2i} = v_{ix}, m_{3i} = v_{iy}, m_{4i} = v_{iz} + \eta_{i}^{2}, m_{5i} = v_{iz}^{2}, m_{6i} = v_{ix}v_{iy}, m_{7i} = v_{iz}^{2}, m_{8i} = (v_{iz}^{2} + \eta_{i}^{2})v_{ix}, m_{9i} = (v_{iz}^{2} + \eta_{i}^{2})v_{iy}, m_{10i} = v_{iz}^{3}, m_{11i} = v_{iz}^{2}v_{iy}, m_{12i} = v_{ix}v_{iz}^{2}, m_{13i} = v_{iz}^{3}, m_{14i} = (v_{iz}^{2} + \eta_{i}^{2})v_{iz}v_{ix}, m_{15i} = (v_{iz}^{2} + \eta_{i}^{2})v_{iz}v_{iy}, m_{16i} = (v_{iz}^{2} + \eta_{i}^{2})v_{iz}^{2}, m_{17i} = \eta_{i}^{2}v_{ix}^{2}, m_{18i} = \eta_{i}^{2}v_{ix}v_{iy}, m_{19i} = \eta_{i}^{2}v_{iz}^{2}, m_{20i} = (v_{iz}^{2} + \eta_{i}^{2})\eta_{i}^{2}, m_{21i} = (v_{iz}^{2} + \eta_{i}^{2})\eta_{i}^{2}v_{ix}, m_{22i} = (v_{iz}^{2} + \eta_{i}^{2})\eta_{i}^{2}v_{iy}, m_{23i} = (v_{iz}^{2} + \eta_{i}^{2})\eta_{i}^{2}v_{ix}, m_{24i} = (v_{iz}^{2} + \eta_{i}^{2})\eta_{i}^{2}v_{iy} \).

Correspondingly, \( \hat{f}_{1}^{eq} = \rho, \hat{f}_{2}^{eq} = \rho u_{x}, \hat{f}_{3}^{eq} = \rho u_{y}, \hat{f}_{4}^{eq} = \rho[(D + I)T + u^2], \hat{f}_{5}^{eq} = \rho(T + u^2), \hat{f}_{6}^{eq} = \rho u_{z}u_{y}, \hat{f}_{7}^{eq} = \rho(T + u^2), \hat{f}_{8}^{eq} = \rho u_{x}[D + I + 2)T + u^2], \hat{f}_{9}^{eq} = \rho u_{x}[(D + I + 2)T + u^2], \hat{f}_{10}^{eq} = \rho[(D + I + 2)T + u^2] + \rho u_{z}^{2}[(D + I + 4)T + u^2], \hat{f}_{11}^{eq} = \rho u_{y}T + \rho u_{z}u_{y}^{2}, \hat{f}_{12}^{eq} = \rho u_{z}T + \rho u_{z}u_{y}^{2}, \hat{f}_{13}^{eq} = 3\rho u_{y}T + \rho u_{y}^{3}, \hat{f}_{14}^{eq} = \rho[(D + I + 2)T + u^2] + \rho u_{z}^{2}[(D + I + 4)T + u^2], \hat{f}_{15}^{eq} = \rho u_{z}u_{y}[(D + I + 4)T + u^2], \hat{f}_{16}^{eq} = \rho[(D + I + 2)T + u^2] + \rho u_{y}^{2}[(D + I + 4)T + u^2], \hat{f}_{17}^{eq} = \rho IT^2 + \rho u_{z}u_{y}IT, \hat{f}_{18}^{eq} = \rho IT^2 + \rho u_{y}^{2}IT, \hat{f}_{19}^{eq} = \rho IT^2 + \rho u_{y}^{2}IT, \hat{f}_{20}^{eq} = \rho IT[u^2 + (D + 3I)T], \hat{f}_{21}^{eq} = \rho u_{x}[u^2 + (D + 2)(D + I + 4)T^2 + (2D + I + 8)u^2T], \hat{f}_{22}^{eq} = \rho u_{y}u^2 + (D + 2)(D + I + 4)T^2 + (2D + I + 8)u^2T], \hat{f}_{23}^{eq} = \rho u_{x}IT[u^2 + (D + 3I + 2)T], \hat{f}_{24}^{eq} = \rho u_{y}IT[u^2 + (D + 3I + 2)T]. \]

Formally, compared with the MRT version of the LBKM for high speed compressible flows \([73, 74]\), the second term, \( C_{i} \), in the right sides of Eq. (11) describes the variation of distribution function due to the chemical reaction. Physically, the present model is based on more moment relations and contains more kinetic information.

The actual combustion procedures are very complicated. In this work we simplify the combustion procedure and present a simple LBKM based on the following assumptions:

1. The flow behavior is described by a single distribution function \( f \). The relaxation coefficient \( R_{k} \) is a constant, where \( k = 1, 2, \ldots, N \).

2. The flow is symmetric, and there are no external forces. The radiative heat loss is neglected.

3. The reaction process is irreversible and described by an empirical or semi-empirical
equation,
\[ \lambda' \frac{d\lambda}{dt} = R(\lambda), \]  \hspace{1cm} (17)
where \( \lambda = \rho_p/\rho \) is the concentration of the reaction product in the system and denotes the progress of the reaction; \( \rho_p \) is the density of the reaction product; \( \rho \) is the density of the whole system.

4. The chemical energy is directly transformed into the internal energy in the following form
\[ \frac{dE}{dt} \bigg|_{R(\lambda)} = \rho Q \lambda' \]  \hspace{1cm} (18)
where \( Q \) is the amount of heat released by the chemical reactant per unit mass.

5. The chemical reaction is slow enough, compared with kinetic procedure of approaching thermodynamic equilibrium, so that
\[ \frac{df}{dt} \bigg|_{R(\lambda)} \approx \frac{df_{eq}}{dt} \bigg|_{R(\lambda)}. \]  \hspace{1cm} (19)
At the same time, it is fast enough, compared with the hydrodynamic flow behavior, so that the chemical reaction results only in the increase of local temperature \( T \) and the local density \( \rho \) and hydrodynamic velocity \( \mathbf{u} \) remain unchanged. Thus,
\[ \frac{df_{eq}}{dt} \bigg|_{R(\lambda)} = \frac{\partial f_{eq}}{\partial T} \frac{dT}{dt} \bigg|_{R(\lambda)}. \]  \hspace{1cm} (20)
The equilibrium distribution function \( f_{eq} \) used here reads
\[ f_{eq} = \rho \left( \frac{1}{2\pi IT} \right)^{D/2} \left( \frac{1}{2\pi IT} \right)^{1/2} \exp \left[ -\frac{(\mathbf{v} - \mathbf{u})^2}{2T} - \frac{\eta^2}{2IT} \right] \]  \hspace{1cm} (21)
which gives
\[ \frac{\partial f_{eq}}{\partial T} = -\frac{(1 + D)IT + I(\mathbf{v} - \mathbf{u})^2 + \eta^2}{2IT^2} f_{eq}. \]  \hspace{1cm} (22)
It is easy to get
\[ \frac{dT}{dt} \bigg|_{R(\lambda)} = \frac{2Q}{D + I} R(\lambda). \]  \hspace{1cm} (23)
from the relation \( E = \rho(D + I)T^2/2 \) and Eqs. (17)-(18). Substituting Eqs. (22)-(23) into (20) gives
\[ C_i = f_{eq}^i Q \frac{(1 + D)IT + I(\mathbf{v}_i - \mathbf{u})^2 + \eta_i^2}{I(D + I)T^2} R(\lambda). \]  \hspace{1cm} (24)
Equations (11) can be rewritten as twenty-four coupled equations in the two-dimensional case. Consequently we need a Discrete Velocity Model (DVM) with at least 24 discrete velocities. To obtain the high computational efficiency, we choose the following two-dimensional
DVM which only has 24 discrete velocities (see Fig.1),

\[ \mathbf{v}_i = \begin{cases} 
(\pm 1,0) & \text{for } 1 \leq i \leq 4, \\
(\pm 1,\pm 1) & \text{for } 5 \leq i \leq 8, \\
& \text{cyc (cyclic permutation)} 
\end{cases} \]  \hspace{1cm} (25)

\[ \mathbf{v}_i = \begin{cases} 
v_a \mathbf{v}_i & \text{for } 1 \leq i \leq 8, \\
v_b \mathbf{v}_{i-8} & \text{for } 8 \leq i \leq 16, \\
v_c \mathbf{v}_{i-16} & \text{for } 17 \leq i \leq 24, 
\end{cases} \]  \hspace{1cm} (26)

\[ \mathbf{v}_i = \begin{cases} 
\eta_a & \text{for } 1 \leq i \leq 8, \\
\eta_b & \text{for } 8 \leq i \leq 16, \\
\eta_c & \text{for } 17 \leq i \leq 24, 
\end{cases} \]  \hspace{1cm} (27)

where cyc indicates the cyclic permutation.

In this work, the spatial derivatives in Eq.(1) are calculated by adopting the NND Nonoscillatory and Nonfree-parameters Dissipative (NND) finite difference scheme [80]. The evolution of chemical process is described by

\[ \frac{\partial \lambda}{\partial t} + u_\alpha \frac{\partial \lambda}{\partial r_\alpha} = \omega_1 p^m (1 - \lambda) + \omega_2 p^n \lambda (1 - \lambda), \]  \hspace{1cm} (28)

where the so-called Cochran’s rate function [81] is adopted for the description of chemical reaction; \( \omega_1, \omega_2, m \) and \( n \) are adjustable parameters. Without losing generality, the ignition temperature \( T_{ig} = 1.1 \) is assumed in this work. Only when \( T > T_{ig} \) can the chemical reaction proceed. And we choose the parameters, \( m = n = 1 \). The temporal derivative in Eq.(28) is solved analytically, and the spatial ones by the NND scheme [80].
The inverse of the matrix $M$ can be analytically solved by the software, Matlab2011. It should be pointed out that, although the complete formulas seems long and complicated, in practical simulations, the parameters $(v_a, v_b, v_c, \eta_a, \eta_b, \eta_c)$ are replaced by specific values, then the elements of matrix $M$ and its inverse $M^{-1}$ are fixed also by specific values before the main loop.

III. CHAPMAN-ENSKOG ANALYSIS OF THE MODEL

The Chapman-Enskog analysis shows that, only if $f^{eq}$ satisfies the statistical relation, (16), or specifically, the eleven equations, (5)-(15), then the LB equation (1) can recover the Navier-Stokes model for combustion. We show the main procedure of the Chapman-Enskog analysis below.

From Eq.(1), we get

$$\frac{\partial \hat{f}}{\partial t} + \frac{\partial}{\partial r}(\hat{E}_\alpha \hat{f}) = -\hat{R}(\hat{f} - \hat{f}^{eq}) + \hat{A} + \hat{C}, \quad (29)$$

where $\hat{C} = M \hat{C}$, $\hat{E}_\alpha = Mv_\alpha M^{-1}$, and $v_\alpha = \text{diag}(v_{1\alpha}, v_{2\alpha}, \cdots, v_{N\alpha})$ is a diagonal matrix.

Expanding the variables with respect to $\varepsilon$ corresponding the Knudsen number, as

$$\begin{align*}
\hat{f}_i &= \hat{f}^{(0)}_i + \hat{f}^{(1)}_i + \hat{f}^{(2)}_i + \cdots, \\
A_i &= A_{1i}, \\
C_i &= C_{1i}, \\
\frac{\partial}{\partial t_l} &= \frac{\partial}{\partial t_1} + \frac{\partial}{\partial t_2}, \\
\frac{\partial}{\partial r_\alpha} &= \frac{\partial}{\partial r_{1\alpha}} \\
&\quad \text{where the part of distribution function } f^{(l)}_i = O(\varepsilon^l), \text{ the modification term } A_{1i} = O(\varepsilon), \\
&\quad \text{the chemical term } C_{1i} = O(\varepsilon), \text{ the partial derivatives } \partial/\partial t_l = O(\varepsilon^l) \text{ and } \partial/\partial r_{1\alpha} = O(\varepsilon), \quad (l = 1, 2, \cdots). \text{ It is easy to get from the first three subequations of Eq.}(30) \text{ that}
\end{align*}$$

$$\hat{f}_i = \hat{f}^{(0)}_i + \hat{f}^{(1)}_i + \hat{f}^{(2)}_i + \cdots, \quad (31)$$

$$\hat{A}_i = \hat{A}_{1i}, \quad (32)$$

$$\hat{C}_i = \hat{C}_{1i}. \quad (33)$$

By substituting the last two subequations of (30) and Eqs.(31)-(33) into (29) and comparing the coefficients of the same order of $\varepsilon$, we have

$$O(\varepsilon^0): \quad \hat{f}^{(0)} = \hat{f}^{eq}, \quad (34)$$


\[ \text{O}(\varepsilon^1): \quad \left( \frac{\partial}{\partial t_1} + \hat{E}_\alpha \frac{\partial}{\partial r_{1a}} \right) \hat{f}^{(0)} = -\hat{R}\hat{f}^{(1)} + \hat{A} + \hat{C}, \quad (35) \]

\[ \text{O}(\varepsilon^2): \quad \frac{\partial}{\partial t_2} \hat{f}^{(0)} + \left( \frac{\partial}{\partial t_1} + \hat{E}_\alpha \frac{\partial}{\partial r_{1a}} \right) \hat{f}^{(1)} = -\hat{R}\hat{f}^{(2)}, \quad (36) \]

where \( f^{(0)} = \left( f_1^{(0)}, f_2^{(0)}, \cdots, f_N^{(0)} \right)^T \). Specifically, \( f^{(0)} \) is the matrix for the equilibria of the moments, \( f^{(1)} \) and \( f^{(2)} \) are the matrices for the first order and second order deviations from equilibria.

From Eq. (35), we get

\[ \frac{\partial \hat{f}_1^{eq}}{\partial t_1} + \frac{\partial \hat{f}_2^{eq}}{\partial x_1} + \frac{\partial \hat{f}_3^{eq}}{\partial y_1} = -R_1 \hat{f}_1^{(1)} + \hat{C}_1, \quad (37) \]

\[ \frac{\partial \hat{f}_2^{eq}}{\partial t_1} + \frac{\partial \hat{f}_5^{eq}}{\partial x_1} + \frac{\partial \hat{f}_6^{eq}}{\partial y_1} = -R_2 \hat{f}_2^{(1)} + \hat{C}_2, \quad (38) \]

\[ \frac{\partial \hat{f}_3^{eq}}{\partial t_1} + \frac{\partial \hat{f}_6^{eq}}{\partial x_1} + \frac{\partial \hat{f}_7^{eq}}{\partial y_1} = -R_3 \hat{f}_3^{(1)} + \hat{C}_3, \quad (39) \]

\[ \frac{\partial \hat{f}_4^{eq}}{\partial t_1} + \frac{\partial \hat{f}_8^{eq}}{\partial x_1} + \frac{\partial \hat{f}_9^{eq}}{\partial y_1} = -R_3 \hat{f}_4^{(1)} + \hat{C}_4, \quad (40) \]

\[ \frac{\partial \hat{f}_5^{eq}}{\partial t_1} + \frac{\partial \hat{f}_10^{eq}}{\partial x_1} + \frac{\partial \hat{f}_11^{eq}}{\partial y_1} = -R_5 \hat{f}_5^{(1)} + \hat{C}_5, \quad (41) \]

\[ \frac{\partial \hat{f}_6^{eq}}{\partial t_1} + \frac{\partial \hat{f}_11^{eq}}{\partial x_1} + \frac{\partial \hat{f}_12^{eq}}{\partial y_1} = -R_6 \hat{f}_6^{(1)} + \hat{C}_6, \quad (42) \]

\[ \frac{\partial \hat{f}_7^{eq}}{\partial t_1} + \frac{\partial \hat{f}_12^{eq}}{\partial x_1} + \frac{\partial \hat{f}_13^{eq}}{\partial y_1} = -R_7 \hat{f}_7^{(1)} + \hat{C}_7, \quad (43) \]

\[ \frac{\partial \hat{f}_8^{eq}}{\partial t_1} + \frac{\partial \hat{f}_14^{eq}}{\partial x_1} + \frac{\partial \hat{f}_15^{eq}}{\partial y_1} = -R_8 \hat{f}_8^{(1)} + \hat{A}_8 + \hat{C}_8, \quad (44) \]

\[ \frac{\partial \hat{f}_9^{eq}}{\partial t_1} + \frac{\partial \hat{f}_15^{eq}}{\partial x_1} + \frac{\partial \hat{f}_16^{eq}}{\partial y_1} = -R_9 \hat{f}_9^{(1)} + \hat{A}_9 + \hat{C}_9, \quad (45) \]

It is easy to get from Eqs. (35)-(13) and (24) that \( \hat{C}_1 = 0, \hat{C}_2 = 0, \hat{C}_3 = 0, \hat{C}_4 = 2\rho \lambda Q, \hat{C}_5 = 2\rho \lambda Q/(D + I), \hat{C}_6 = 0, \hat{C}_7 = 2\rho \lambda Q/(D + I), \hat{C}_8 = 2\rho u_x \lambda Q(D + I + 2)/(D + I), \hat{C}_9 = 2\rho u_y \lambda Q(D + I + 2)/(D + I) \). Substituting the all the specific forms of \( \hat{C}_i \) and \( \hat{f}_i^{eq} \) into (37)-(45) gives

\[ \frac{\partial \hat{p}}{\partial t_1} + \frac{\partial \hat{j}_x}{\partial x_1} + \frac{\partial \hat{j}_y}{\partial y_1} = 0, \quad (46) \]

\[ \frac{\partial \hat{j}_x}{\partial t_1} + \frac{\partial \rho(T + u_x^2)}{\partial x_1} + \frac{\partial \rho u_x u_y}{\partial y_1} = 0, \quad (47) \]
Adding Eqs.(46)-(49) and (55)-(58) leads to the following equations,

\[
\frac{\partial j_x}{\partial t} + \frac{\partial \rho u_x u_y}{\partial x} + \frac{\partial (T + u_y^2)}{\partial y} = 0, \tag{48}
\]

\[
\frac{\partial j_y}{\partial t} + \frac{\partial \rho u_x u_y}{\partial x} + \frac{\partial (T + u_x^2)}{\partial y} = 0, \tag{49}
\]

\[
\frac{\partial \rho (T + u_x^2)}{\partial t} + \frac{\partial \rho (3u_x T + u_x^2)}{\partial x} + \frac{\partial (u_x T + u_x u_y^2)}{\partial y} = -R_s \dot{f}_5^{(1)} + \rho \lambda' Q \frac{2}{D + I}, \tag{50}
\]

\[
\frac{\partial \rho u_x [D + I + 2] T + u^2}{\partial t} + \frac{\partial}{\partial x} \left\{ \rho [(D + I + 2) T + u^2] T + \rho u_x (D + I + 4) T + u^2 \right\}
+ \frac{\partial \rho u_x u_y [D + I + 4] T + u^2}{\partial y} = -R_s \dot{f}_8^{(1)} + \dot{A}_8 + 2 \rho u_x \lambda' Q \frac{D + I + 2}{D + I}, \tag{53}
\]

\[
\frac{\partial \rho u_y [D + I + 2] T + u^2}{\partial t} + \frac{\partial}{\partial y} \left\{ \rho [(D + I + 2) T + u^2] T + \rho u_y (D + I + 4) T + u^2 \right\}
+ \frac{\partial \rho u_x u_y [D + I + 4] T + u^2}{\partial x} = -R_s \dot{f}_7^{(1)} + \dot{A}_9 + 2 \rho u_y \lambda' Q \frac{D + I + 2}{D + I}, \tag{54}
\]

where \( j_x = \rho u_x, j_y = \rho u_y, \) and \( \xi = (D + I) \rho T + (j_x^2 + j_y^2)/\rho \) is twice the total energy.

From Eq.(36), we get

\[
\frac{\partial \rho}{\partial t} = 0, \tag{55}
\]

\[
\frac{\partial j_x}{\partial t} + \frac{\partial \dot{f}_5^{(1)}}{\partial x} + \frac{\partial \dot{f}_6^{(1)}}{\partial y} = 0, \tag{56}
\]

\[
\frac{\partial j_y}{\partial t} + \frac{\partial \dot{f}_6^{(1)}}{\partial x} + \frac{\partial \dot{f}_7^{(1)}}{\partial y} = 0, \tag{57}
\]

\[
\frac{\partial \xi}{\partial t} + \frac{\partial \dot{f}_8^{(1)}}{\partial x} + \frac{\partial \dot{f}_9^{(1)}}{\partial y} = 0. \tag{58}
\]

Adding Eqs.(46)-(49) and (55)-(58) leads to the following equations,

\[
\frac{\partial j_x}{\partial t} + \frac{\partial \rho (T + u_x^2)}{\partial x} + \frac{\partial \rho u_x u_y}{\partial y} + \frac{\partial \dot{f}_5^{(1)}}{\partial x} + \frac{\partial \dot{f}_6^{(1)}}{\partial y} = 0, \tag{59}
\]

\[
\frac{\partial j_y}{\partial t} + \frac{\partial \rho (T + u_y^2)}{\partial y} + \frac{\partial \rho u_x u_y}{\partial x} + \frac{\partial \dot{f}_7^{(1)}}{\partial x} + \frac{\partial \dot{f}_6^{(1)}}{\partial y} = 0, \tag{60}
\]

\[
\frac{\partial j_x}{\partial t} + \frac{\partial \rho (T + u_x^2)}{\partial x} + \frac{\partial \rho u_x u_y}{\partial y} + \frac{\partial \dot{f}_7^{(1)}}{\partial x} + \frac{\partial \dot{f}_8^{(1)}}{\partial y} = 0, \tag{61}
\]
\[
\frac{\partial \xi}{\partial t} + \frac{\partial p}{\partial x} \frac{\partial T}{\partial x} + \frac{\partial p}{\partial y} \frac{\partial T}{\partial y} + \frac{\partial f_{1}}{\partial x} + \frac{\partial f_{2}}{\partial y} = 2\rho \lambda' Q, \tag{62}
\]

From Eqs. (50)-(54) and (59)-(62), we finally obtain the Navier-Stokes equations:

\[
\frac{\partial p}{\partial t} + \frac{j_{x}}{\partial x} + \frac{j_{y}}{\partial y} = 0, \tag{63}
\]

\[
= \frac{\partial}{\partial x} \left[ \rho T \frac{\partial u_{x}}{\partial x} - \frac{2}{D + I} \frac{\partial u_{x}}{\partial x} - \frac{2}{D + I} \frac{\partial u_{y}}{\partial y} \right] + \frac{\partial}{\partial y} \left[ \rho T \frac{\partial u_{y}}{\partial y} - \frac{2}{D + I} \frac{\partial u_{y}}{\partial y} - \frac{2}{D + I} \frac{\partial u_{y}}{\partial y} \right], \tag{64}
\]

\[
= \frac{\partial}{\partial x} \left[ \rho T \frac{\partial u_{x}}{\partial x} + \frac{2}{D + I} \frac{\partial u_{y}}{\partial x} + \frac{2}{D + I} \frac{\partial u_{y}}{\partial y} \right] + \frac{\partial}{\partial y} \left[ \rho T \frac{\partial u_{y}}{\partial y} + \frac{2}{D + I} \frac{\partial u_{y}}{\partial y} + \frac{2}{D + I} \frac{\partial u_{y}}{\partial y} \right], \tag{65}
\]

\[
= 2 \frac{\partial}{\partial x} \left[ \rho T \frac{\partial u_{x}}{\partial x} - \frac{2}{D + I} \frac{\partial u_{x}}{\partial x} - \frac{2}{D + I} \frac{\partial u_{y}}{\partial y} \right] - \frac{\partial}{\partial y} \left[ \rho T \frac{\partial u_{y}}{\partial y} - \frac{2}{D + I} \frac{\partial u_{y}}{\partial y} - \frac{2}{D + I} \frac{\partial u_{y}}{\partial y} \right] - \frac{1}{2} \frac{\tilde{A}_{8}}{R_{8}} + 2 \frac{\partial}{\partial y} \left[ \rho T \frac{\partial u_{y}}{\partial y} - \frac{2}{D + I} \frac{\partial u_{y}}{\partial y} - \frac{2}{D + I} \frac{\partial u_{y}}{\partial y} \right] - \frac{1}{2} \frac{\tilde{A}_{9}}{R_{9}} \tag{66}
\]

Here \( c_{p} = (D + I + 2)/2 \) is the specific-heat at constant pressure. The specific-heat at constant volume can be defined as \( c_{v} = (D + I)/2 \). Substituting Eqs. (3) and (4) into the above equation (66) gives

\[
= 2 \frac{\partial}{\partial x} \left[ \rho T \frac{\partial u_{x}}{\partial x} - \frac{2}{D + I} \frac{\partial u_{x}}{\partial x} - \frac{2}{D + I} \frac{\partial u_{y}}{\partial y} \right] - \frac{\partial}{\partial y} \left[ \rho T \frac{\partial u_{y}}{\partial y} - \frac{2}{D + I} \frac{\partial u_{y}}{\partial y} - \frac{2}{D + I} \frac{\partial u_{y}}{\partial y} \right] + 2 \frac{\partial}{\partial y} \left[ \rho T \frac{\partial u_{y}}{\partial y} - \frac{2}{D + I} \frac{\partial u_{y}}{\partial y} - \frac{2}{D + I} \frac{\partial u_{y}}{\partial y} \right] \tag{67}
\]

It is clear to find that, by substituting the specific form of \( \tilde{A}_{8} \) and \( \tilde{A}_{9} \) into Eq. (67), the viscous coefficient in the energy equation (67) is consistent with that in the momentum equation.
Up to this step, we can find that the proposed MRT-LBKM recover the consistent Navier-Stokes equations in the hydrodynamic limit.

More discussions are as below. The coefficient $\hat{R}$ represents the inverse of the relaxation time from $\hat{f}$ to its equilibrium $\hat{f}^{eq}$. $\hat{f}_1 = \hat{f}_1^{eq}$, $\hat{f}_2 = \hat{f}_2^{eq}$, $\hat{f}_3 = \hat{f}_3^{eq}$, $\hat{f}_4 = \hat{f}_4^{eq}$. Consequently, the values of $R_1$, $R_2$, $R_3$, $R_4$ have no influence on the LB evolution. Furthermore, the relaxation parameters $R_i$ are not completely independent for the system with isotropy constraints. Specifically, $R_5$, $R_6$, $R_7$ are related to viscosity, and the viscosity coefficient is $\mu = \rho T/R_\mu$ when $R_5 = R_6 = R_7 = R_\mu$; $R_8$, $R_9$ are related to heat conductivity, and the heat conductivity coefficient is $\kappa = c_p \rho T/R_\kappa$ when $R_8 = R_9 = R_\kappa$. Consequently, both the specific-heat ratio,

$$\gamma = \frac{c_p}{c_v} = \frac{D + I + 2}{D + I},$$

and the Prandtl number,

$$Pr = \frac{c_p \mu}{\kappa} = \frac{R_\kappa}{R_\mu},$$

are flexible in this model. When $R_5 = R_6 = R_7 = R_\mu$, $R_8 = R_9 = R_\kappa$, the above Navier-Stokes equations reduce to

$$\frac{\partial \rho}{\partial t} + \frac{\partial j_\alpha}{\partial r_\alpha} = 0,$$

$$\frac{\partial j_\alpha}{\partial t} + \frac{\partial p}{\partial r_\alpha} + \frac{\partial \rho u_\alpha u_\beta}{\partial r_\beta} = -\frac{\partial P_{\alpha\beta}}{\partial r_\beta},$$

$$\frac{\partial \xi}{\partial t} + \frac{\partial (\xi + 2p)u_\alpha}{\partial r_\alpha} = 2\rho \chi'Q + 2\frac{\partial}{\partial r_\beta} \left( \frac{\partial T}{\partial r_\beta} - P_{\alpha\beta} u_\alpha \right)$$

where

$$\mu_B = \mu \left( \frac{2}{3} - \frac{2}{D + I} \right),$$

$$P_{\alpha\beta} = -\mu \left( \frac{\partial u_\alpha}{\partial r_\beta} + \frac{\partial u_\beta}{\partial r_\alpha} - \frac{2}{3} \frac{\partial u_\chi}{\partial r_\chi} \delta_{\alpha\beta} \right) - \mu_B \frac{\partial u_\alpha}{\partial r_\chi} \delta_{\alpha\beta}.$$

Specifically, $P_{xx} = \hat{f}_5^{(1)}$, $P_{xy} = P_{yx} = \hat{f}_6^{(1)}$, $P_{yy} = \hat{f}_7^{(1)}$.

**IV. NUMERICAL TESTS OF THE MODEL**

To validate and verify the newly proposed LB kinetic model, here we show simulation results of some well-known benchmark numerical examples which include one for the steady detonation, three for the Riemann problems, one for the shock reflection and one for the Couette flow. The parameter for chemical reaction heat $Q$ is not zero only for the first
FIG. 2: (Color online) The profile of the steady detonation: (a) $\rho$, (b) $T$, (c) $p$, (d) $u_x$, (e) $\lambda$. Numerical test. For the cases with the Couette flow, results with different specific heat ratios and Prandtl numbers are shown.

A. Steady detonation

As the first numerical test, a one-dimensional steady detonation is simulated here to validate our model. The initial physical quantities are:

\[
\begin{align*}
\{ & (\rho, T, u_x, u_y, \lambda)_L = (1.38837, 1.57856, 0.577350, 0, 1) \\
& (\rho, T, u_x, u_y, \lambda)_R = (1, 1, 0, 0, 0) \}
\]

(75)

where the suffixes $L$ and $R$ index two parts, $0 \leq x \leq 0.2$ and $0.2 < r \leq 1$, respectively. Here we choose $v_a = 2.7$, $v_b = 2.2$, $v_c = 1.2$, $\eta_a = 5$, $\eta_b = 3$, $\eta_c = 1.1$, $I = 3$, $\Delta t = 5 \times 10^{-6}$, $\Delta x = \Delta y = 2 \times 10^{-4}$, $Q = 1$. The collision parameters in MRT are $R_5 = R_6 = R_7 = 10^4$ and $10^5$ for the others. Figure 2 shows the profile of the steady detonation at time $t = 0.39$. Panels (a)-(e) gives physical quantities $\rho, T, P, u_x, \lambda$ versus $x$, respectively. The simulation results of LB, analytic solutions of CJ theory \[18, 19, 23\] and ZND theory \[20, 23\] are shown is each panel. The solid lines with squares, the dashed lines and the solid lines are for LB simulation results, CJ results and ZND results, respectively. The simulation results give physical quantities behind the detonation wave $(\rho, T, u_x, u_\theta, \lambda) = (1.38869, 1.57816, 0.577384, 0, 1)$. 

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FIG. 3: (Color online) The profile of $p$ in the evolution of the steady detonation at times $t = 0.29$, $t = 0.34$, $t = 0.39$, respectively.

Comparing them with CJ results gives the relative differences 0.023%, 0.025%, 0.006%, 0% and 0%, respectively. It is clear in panels (a)-(e) that the LB simulation results agree well with the ZND results in the area behind von Neumann peak. But there exist significant difference in front of the von Neumann peaks. This is because the ZND theory used here ignores completely the effects of viscosity and heat conduction, and the von Neumann peak is treated simply as a strong discontinuity which is not true. While in the LB results the effects of viscosity, heat conduction and other kinds of relevant transportation are included. This difference will decrease with the decreasing of viscosity and heat conductivity. This point will be further discussed in section V.

Figure 4 shows the pressure versus $x$ at times $t = 0.29$, $t = 0.34$, $t = 0.39$, from left to right, respectively. Our simulation gives detonation velocity $v_D = 2.06$, and the analytic solution is $v_D = 2.06395$. The relative difference between them is 0.191% which is satisfying.

B. Riemann problems

In this subsection our two-dimensional LB model is used to solve the one-dimensional Riemann problems where there is no chemical reaction. Now we give simulation results for three typical Riemann problems, i.e., the Sod’s shock tube, the Lax’s shock tube and the Sjogreen’s problem.
FIG. 4: (Color online) Comparison of numerical and theoretical results for the Sod shock tube at $t = 0.2$. Solid lines are for exact solutions and solid lines with squares are for simulation results.

1. Sod’s shock tube

For the problem of Sod’s shock tube, the initial condition is described by

$$\begin{cases} (\rho, T, u_x, u_y)_L = (1, 1, 0, 0) \\ (\rho, T, u_x, u_y)_R = (0.125, 0.8, 0, 0) \end{cases} \tag{76}$$

where left side $L \in [0, 0.5)$ and the right side $R \in [0.5, 1]$. Figure 7 shows the computed density, temperature, pressure, velocity profiles at the time $t = 0.2$. The lines are for analytical solutions and solid lines with squares are for the LB simulation results. The size of grid is $\Delta x = \Delta y = 10^{-3}$, time step $\Delta t = 10^{-5}$, $I = 3$ and $\left( v_a, v_b, v_c, \eta_a, \eta_b, \eta_c \right) = (2.5, 2.2, 1.2, 6.5, 3, 0)$. The collision parameters in MRT are $R_5 = R_6 = R_7 = 1.2 \times 10^4$, and other values of $R_i$ are $10^5$. It is easy to find in Fig.4 that the two sets of results have a satisfying agreement.

2. Lax’s shock tube

For this problem, the initial condition is described by

$$\begin{cases} (\rho, T, u_x, u_y)_L = (0.445, 7.928, 0.698, 0) \\ (\rho, T, u_x, u_y)_R = (0.5, 1.142, 0, 0) \end{cases} \tag{77}$$

where $L \in [-1, 0)$ and $R \in [0, 1]$. Figure 5 shows the physical quantities (density, temperature, pressure, velocity) versus $x$ at the time $t = 0.15$. The lines are for exact solutions and solid lines with squares correspond to our simulation results. The parameters are set to be $\Delta x = \Delta y = 10^{-3}$, $\Delta t = 10^{-5}$, $I = 1$, $\left( v_a, v_b, v_c, \eta_a, \eta_b, \eta_c \right) = (4.7, 3.3, 1, 6, 2.5, 0.9)$. The
collision parameters in MRT are \( R_5 = R_6 = R_7 = 2 \times 10^4 \), \( R_8 = R_9 = 8 \times 10^4 \), and other values of \( R_i \) are \( 10^5 \). We also find a good agreement between the two sets of results.

3. Sjogren’s problem

The initial condition for the Sjogren’s problem is

\[
\begin{align*}
(\rho, T, u_x, u_y)_L &= (1.0, 0.5, -1.2, 0) \\
(\rho, T, u_x, u_y)_R &= (1.0, 0.5, 1.2, 0)
\end{align*}
\]

(78)

where \( L \in [-0.5, 0] \) and \( R \in [0, 0.5] \). Figure 5 shows the physical quantities versus \( x \) at the time \( t = 0.03 \). The specific correspondences are referred to the legends. The parameters used here are \( \Delta x = \Delta y = 2 \times 10^{-3} \), \( \Delta t = 2 \times 10^{-5} \), \( I = 4 \), \( (v_a, v_b, v_c, \eta_a, \eta_b, \eta_c) = (0.4, 1.0, 1.8, 0.3, 1.9, 1.5) \). The collision parameters in MRT are \( R_8 = R_9 = 2 \times 10^4 \), and others \( 5 \times 10^4 \). We also find a good agreement between the two sets of results.
FIG. 7: Density contour of steady regular shock reflection on a wall at $t = 0.5$. From black to white, the density increases.

C. Shock reflection

In this test, an incoming shock wave with Mach number 2.3094 has an angle of $30^\circ$ to the wall. The computational domain is a rectangle with length 0.3 and height 0.1. This domain is divided into a $300 \times 100$ rectangular grid with $\Delta x = \Delta y = 10^{-3}$. The boundary conditions are composed of a reflecting surface along the bottom boundary, supersonic outflow along the right boundary, and Dirichlet conditions on the left and top boundary conditions, given by

$$
\begin{align*}
(p, T, u_x, u_y)_{0,y,t} &= (1, 0.5, 2, 0) \\
(p, T, u_x, u_y)_{x,0.1,t} &= (1.25, 0.56, 1.9, -0.173205)
\end{align*}
$$

The parameters are chosen as $\Delta t = 5 \times 10^{-6}$, $I = 2$, $(v_a, v_b, v_c, \eta_a, \eta_b, \eta_c) = (1.0, 2.7, 2.9, 1.0, 2.9, 0.96)$. The collision parameters in MRT are $R_5 = R_6 = R_7 = 1.8 \times 10^5$, $R_8 = R_9 = 2.0 \times 10^5$, and other values of $R_i$ are $10^5$. Figure 7 shows contours of density at $t = 0.5$. The clear shock reflection on the wall agrees well with the exact solution.

D. Couette Flow

In order to demonstrate that the new model is also suitable for incompressible flows, we conduct a series of numerical simulations of Couette flow. The upper wall, with the distance $H = 0.2$ apart from the lower wall, moves with a fixed speed $u_0$. The lower wall is at rest. Periodic boundary conditions are applied to the left and right boundaries, and the top and bottom adopt the nonequilibrium extrapolation method.

In the first simulation of Couette flow, the initial state of the fluid is $\rho = 1$, $T = 1$, $u_x = u_y = 0$. The viscous shear stress transmits momentum into the fluid and changes the horizontal speed profile. Figure 8 shows the horizontal speed distribution at various
FIG. 8: (Color online) Horizontal speed distribution of Couette flow at various instants: \( t = 1, t = 5, t = 30 \).

FIG. 9: (Color online) Temperature profiles of Couette flow. (a) \( \gamma = 1.4 \). (b) \( \gamma = 1.5 \)

instants \( t = 1, 5, 30 \). The simulation results coincide well with the following analysis,

\[
 u = \frac{y}{H} u_0 + \frac{2}{\pi} u_0 \sum_{n=1}^{\infty} \left[ \frac{(-1)^n}{n} \exp(-n^2 \pi^2 \frac{\mu t}{\rho H^2}) \sin\left(\frac{n\pi y}{H}\right) \right] \tag{80}
\]

The parameters are \( \Delta x = 10^{-3}, \Delta t = 10^{-5}, I = 2, (v_a, v_b, v_c, \eta_a, \eta_b, \eta_c) = (0.8, 1.2, 1.3, 1.0, 2.7, 0.8) \). The grid number is \( N_x \times N_y = 1 \times 200 \). The collision parameters are \( R_5 = R_6 = R_7 = 2 \times 10^3, R_8 = R_9 = 1.0 \times 10^4 \), and the others \( 5 \times 10^4 \).

Figure 9 shows the temperature profiles in another four simulations. In order to get a steady fluid state as soon as possible, we give the initial temperature field as below

\[
 T = T_1 + (T_2 - T_1) \frac{x}{H} + \frac{\mu}{2\kappa} u_0^2 \frac{x}{H} (1 - \frac{x}{H}) \tag{81}
\]

where \( T_1 (= 1.0) \) and \( T_2 (= 1.01) \) are temperatures of the lower and upper walls, respectively. The initial velocity field is given as \( u = u_0 y/H \). And the time is \( t = 0.01 \). Panels (a)-(b) correspond to \( \gamma = 1.4 \) and \( \gamma = 1.5 \), respectively. The case \( Pr = 0.2 \) in panel (a) corresponds to \( \Delta x = 10^{-3}, \Delta t = 10^{-5}, I = 3, (v_a, v_b, v_c, \eta_a, \eta_b, \eta_c) = (0.8, 1.2, 1.3, 1.1, 3.1, 0.7) \), \( R_5 = R_6 = R_7 = 10^4, R_8 = R_9 = 2 \times 10^3, R_{21} = R_{22} = R_{23} = R_{24} = 10^3 \), and \( 5 \times 10^4 \) for other collision parameters. For the case \( Pr = 5.0 \) in panel (a), the parameters are \( \eta_c = 0.7, \)
\[ R_5 = R_6 = R_7 = 2 \times 10^3, \quad R_8 = R_9 = 10^4, \quad R_{21} = R_{22} = R_{23} = R_{24} = 5 \times 10^4, \text{ and the others are the same as those for } Pr = 0.2 \text{ in panel (a). Except } I = 2 \text{ and } \eta_b = 2.1, \text{ all the other parameters for the cases } Pr = 0.2 \text{ and } Pr = 5.0 \text{ in panel (b) are the same as those for the cases } Pr = 0.2 \text{ and } Pr = 5.0 \text{ in panel (a), respectively. It is clear that our simulation results are in agreement with the analytical ones, and the effects of the specific-heat ratio and the Prandtl number are successfully captured.}

V. NONEQUILIBRIUM INVESTIGATION OF DETONATION

The LB kinetic model inherits naturally the function of Boltzmann equation, describing nonequilibrium effects in the system \[32, 43, 67, 75–78\]. The departure of the system from local thermodynamic nonequilibrium can be measured by the difference between the high order moments of \( f_i \) and \( f_i^{eq} \) which are just \( (\hat{f}_k - \hat{f}_k^{eq}) \) in the current MRT-LB kinetic equation, †. We define

\[ \Delta_k = \hat{f}_k - \hat{f}_k^{eq}. \] (82)

It is easy to find that \( \Delta_k = 0 \) for \( k = 1, 2, 3, 4 \) due to the conservation of mass, momentum and energy. Each non-zero \( \Delta_k \) quantitatively describes the deviation state of the system from its local thermodynamic equilibrium from its own side. We can observe the thermodynamic nonequilibrium state in the \( N \)-dimensional space opened by \( \Delta_k \) with \( k = 1, 2, \cdots, N \). We further define a distance

\[ d = \sqrt{\sum_{k=1}^{N} \Delta_k^2}, \] (83)

which is a rough and averaged estimation of the deviation amplitude from the thermodynamic equilibrium, where \( \Delta_k \) is assumed to be dimensionless. Thus, \( d = 0 \) when the system is in the thermodynamic equilibrium and \( d > 0 \) in the thermodynamic nonequilibrium state.

In this part we give some results of \( \Delta_k \) in the evolution of detonation. Corresponding to the simple definition of \( \Delta_k \), we introduce some clear symbols as \( \Delta_{v_x v_x} = \Delta_5, \Delta_{v_x v_y} = \Delta_6, \Delta_{v_y v_y} = \Delta_7, \Delta_{\eta^2} = \Delta_4 - \Delta_5 - \Delta_7, \Delta_{(v^2 + \eta^2)v_x} = \Delta_8, \Delta_{(v^2 + \eta^2)v_y} = \Delta_9, \Delta_{v_x v_x v_x} = \Delta_{10}, \Delta_{v_x v_x v_y} = \Delta_{11}, \Delta_{v_x v_y v_y} = \Delta_{12}, \Delta_{v_y v_y v_y} = \Delta_{13} \).

A short discussion is as below. The nonequilibrium behaviors of various modes may contribute to the system evolution according to different amplification factors \( R_k \), while all the amplification factors becomes the same in the SRT-LB model. Mathematically, the part
$R_k \Delta_k$ in the right side of Eq. (29) increases with increasing $R_k$ and fixed $\Delta_k$.

A. Simulation with different space and time steps

Now we investigate some nonequilibrium behaviors in detonation phenomena. The initial physical quantities ($\rho, T, u_x, u_y, \lambda$) are given the same values as those in Eq. (75). Here we choose $v_a = 2.7$, $v_b = 2.2$, $v_c = 1.2$, $\eta_a = 1.5$, $\eta_b = 0.5$, $\eta_c = 5.0$, $I = 3$, $Q = 1$. The collision parameters in MRT are $R_i = 100$. In numerical simulations the space and time steps should be small enough so that the spurious transportation is negligible compared with the physical one [78]. To assure that the numerical errors are small enough, we simulate the detonation in three cases with different space and time steps: (i) $\Delta x = \Delta y = 10^{-3}$, $\Delta t = 10^{-5}$; (ii) $\Delta x = \Delta y = 10^{-3}$, $\Delta t = 10^{-6}$; (iii) $\Delta x = \Delta y = 10^{-4}$, $\Delta t = 10^{-6}$.

Figure 10 shows the simulation results of physical quantities ($\rho$, $T$, $p$, $u_x$, $u_y$, $\lambda$, $\eta^2$, $\Delta v_x v_y$, $\Delta v_y v_y$, $\Delta v_x v_x$, $\Delta v_x v_y$, $\Delta v_y v_x$, $\Delta v_y v_y$, $\Delta (v^2+\eta^2)v_x$, $\Delta (v^2+\eta^2)v_y$) versus $x$ at time $t = 0.35$ in the three cases. A vertical dashed guideline is plotted in each panel to guide the eye for the horizontal position $x = 0.8345$ corresponding to the peak of pressure.

(1) The detonation shown in Fig. 10 is not a steady one at time $t = 0.35$. The pressure at the von-Neumann-peak will increase further. While the detonation shown in Fig. 3 is already steady at the time $t = 0.35$. Physically, the viscosity of the physical system in Fig. 10 is much larger than that in Fig. 3. It takes more time for a steady detonation wave to form as the viscosity increases.

(2) The simulation results of each quantity in the three cases coincide well. It shows that all the above calculation results are valid. On the one hand, the grid size 0.001 and the time step $10^{-5}$ in the first case is already small enough to get much exact simulation results for the current problem. On the other hand, all the simulation results given in panels (a)-(o) are physically valid. Given $R_i$ small enough, the physical viscosity is much larger than numerical viscosity here.

(3) Panels (a)-(d) show that the maximum values of density, temperature, pressure, velocity are not located at the same $x$-coordinate. Here we define the von-Neumann-peak as the point where the largest pressure is. It can be found in panel (e) that the peak is located in the reaction zone where $0 < \lambda < 1$.

(4) As shown in panels (f), (h), (i), the simulation results of $\Delta v_x v_x$, $\Delta v_y v_y$ and $\Delta \eta^2$ satisfy
FIG. 10: (Color online) Physical quantities versus $x$ at time $t = 0.35$ in three cases: (a) $\rho$, (b) $T$, (c) $p$, (d) $u_x$, (e) $\lambda$, (f) $\Delta u_x u_y$, (g) $\Delta v_x v_y$, (h) $\Delta u_y v_y$, (i) $\Delta_{\eta^2}$, (j) $\Delta_{v_x v_x v_x}$, (k) $\Delta_{v_x v_y v_y}$, (l) $\Delta_{v_y v_y}$, (m) $\Delta_{v_y v_y}$, (n) $\Delta_{(\eta^2+\eta^2)v_x}$, (o) $\Delta_{(\eta^2+\eta^2)v_y}$. 
the relation \( \Delta v_x v_x + \Delta v_y v_y + \Delta \eta^2 = 0 \). Physically, when the system is not in its thermodynamic equilibrium state, the so-called internal energy in different degrees of freedom may not equal each other. The exchange of the internal energy in different degrees of freedom, due to the molecule collision, makes them tend toward their average. The relaxation coefficients \( R_5 \) and \( R_7 \) are related to the internal energy in \( x \) and \( y \) degree of freedom, respectively. The departures of the internal energy in different degrees of freedom from their average are described by \( \Delta v_x v_x \), \( \Delta v_y v_y \) and \( \Delta \eta^2 \) here. The simulation results of \( \Delta v_x v_x \), \( \Delta v_y v_y \) and \( \Delta \eta^2 \) are not equal to zero around the detonation wave, where the system is nonequilibrium and the energy equipartition theory breaks down.

(5) Both \( \Delta v_x v_x \) and \( \Delta \eta^2 \) show a crest and a trough in the reaction zone, and \( \Delta v_y v_y \) shows a crest and two troughs. The result of \( \Delta v_x v_x \) first shows a crest and then a trough when the detonation wave travels forward. While \( \Delta \eta^2 \) show an opposite behavior. And the crest of \( \Delta v_y v_y \) is between its two troughs. Physically, comparing with the internal energy in the \( y \) or extra degree of freedom, the internal energy in the \( x \) degree of freedom first increases in the preshocked area. And the maximum absolute value of \( \Delta v_x v_x \) is the largest among \( \Delta v_x v_x \), \( \Delta v_y v_y \) and \( \Delta \eta^2 \) in the whole system.

(6) Panels (g), (k), (m), (o) show that the results of \( \Delta v_x v_y \), \( \Delta v_x v_x v_y \), \( \Delta v_y v_y v_y \), \( \Delta (v^2 + \eta^2) v_y \) are equal to zero. Physically, \( \Delta v_x v_y \) associates with the shear effect, \( \Delta v_x v_x v_y \), \( \Delta v_y v_y v_y \), \( \Delta (v^2 + \eta^2) v_y \) are related to “the internal energy flow caused by microscopic fluctuation” in \( y \) direction. Because the simulated system is symmetrical in \( y \) direction. There is neither shear effect nor energy flux in \( y \) direction. This is the reason why \( \Delta v_x v_y = 0 \) and \( \Delta v_x v_x v_y = \Delta v_y v_y v_y = \Delta (v^2 + \eta^2) v_y = 0 \) in the current case.

(7) It can be found in panels (j), (l), (n) that \( \Delta v_x v_x v_x \), \( \Delta v_x v_y v_y \), \( \Delta (v^2 + \eta^2) v_x \) are not close to zero. Physically, \( \Delta v_x v_x v_x \), \( \Delta v_x v_y v_y \), \( \Delta (v^2 + \eta^2) v_x \) are associated with “the internal energy flow caused by microscopic fluctuation” in \( x \) direction. The compression and rarefaction play roles on the system successively, with chemical energy released continuously in the reaction zone. Those effects make the velocity distribution function asymmetrical about the point \( (v_x = u_x, v_y = u_y) \) which is the symcenter of the Maxwellian distribution (see Eq. \( \text{(21)} \)). This is the fundamental reason why \( \Delta v_x v_x v_x \), \( \Delta v_x v_y v_y \) are not close to zero in the reaction zero.
FIG. 11: (Color online) The physical quantities $p$ and $\Delta v_x v_x$ versus $x$ at time $t = 0.35$. The first row is for the pressure and the second for $\Delta v_x v_x$. From left to right, the three columns are for $R_i = 10^2$, $R_i = 10^3$ and $R_i = 10^4$, respectively.

B. Investigation with different collision parameters

Now we give and compare three simulations of detonation phenomena with different collision parameter: (i) $R_i = 10^2$, (ii) $R_i = 10^3$, (iii) $R_i = 10^4$. The first case is case (i) in the above subsection. In the case $R_i = 10^3$, the parameters $(v_a, v_b, v_c, \eta_a, \eta_b, \eta_c) = (2.7, 2.6, 1.9, 5.0, 0.0, 1.7)$, $\Delta x = 2 \times 10^{-4}$, $\Delta t = 2 \times 10^{-6}$, the other parameters are the same as the first case. In the case $R_i = 10^4$, the spacial and temporal steps $\Delta x = 4 \times 10^{-5}$, $\Delta t = 4 \times 10^{-6}$, the other parameters are the same as the second one.

Figure 11 shows the simulation results of $p$ and $\Delta v_x v_x$ versus $x$ at time $t = 0.35$ in the three cases with $R_i = 10^2$, $R_i = 10^3$ and $R_i = 10^4$, respectively. Here we define $(X_m, P_m)$ as the point where the largest pressure is located. The points in panels (a)-(c) are $(0.83450, 2.39850)$, $(0.86410, 3.01965)$ and $(0.87906, 3.33212)$, respectively. A vertical dashed guideline is plotted across this point in each panel. Aside this guideline, another two lines are given to guide the eye for the width of the detonation wave. At the right side of the rightmost line is the unreacted explosive in metastable equilibrium with zero reaction rate. At the left side of the leftmost line is a constant state. The detonation wave is in nonequilibrium. The guidelines in panels (d)-(f) coincide with those in (a)-(c), respectively.
(1) It is clear to find in panels (a)-(f) that the detonation wave, especially the preshocked area, becomes narrower with increasing $R_i$. Physically, the viscosity which is inversely proportional to $R_\mu$ widens the detonation wave, especially the preshocked area. Correspondingly, the area of nonequilibrium system is widened as well.

(2) Panels (a)-(c) show that both $X_m$ and $P_m$ increase from left to right. That is to say, with the increase of $R_i$, it takes less time for the detonation to become steady, and the von Neumann peaks becomes sharper. Physically, the viscosity smooths wave front of pressure.

(3) In panels (d)-(f), the shaded area enclosed by the curve $\Delta v_x v_x (x)$ and the line $\Delta v_x v_x = 0$ decreases from left to right. This shaded area could describe the nonequilibrium effect of detonation wave in the system. From this aspect, the viscosity increases the nonequilibrium.

(4) The minimum of $\Delta v_x v_x$ is $-0.06759$, $-0.07018$, $-0.01275$ in panels (d)-(f), respectively. The corresponding maximum is $0.34753$, $0.40275$, $0.40857$, respectively. The minimum of $\Delta v_x v_x$ for $R = 1000$ is less than the other two, and the maximum for $R = 10000$ is the largest among the three cases. In fact, there is competition between the viscosity effect, the thermal diffusion effect and the gradient effects of physical quantities ($\rho$, $u$, $T$, $p$, etc.). With the increase of collision parameters, the heat conductivity reduces and the gradients of physical quantities increase, which enhances the nonequilibrium effect. While the decrease of viscosity which is inversely proportional to $R_\mu$ weakens this effect.

(5) The horizontal position for $\Delta v_x v_x = 0$ in the detonation wave moves towards the horizontal position for the von Neumann peak as $R_i$ increases. It can be found a clear distance from the position for $\Delta v_x v_x = 0$ to the position for the von Neumann peak in panel (a). While they almost coincide in (c). That is to say, the position where the internal energy in the $x$ degree of freedom equals the average of all degrees of freedom gets away from the position for the von Neumann peak with increasing viscosity.

VI. SUMMARY AND CONCLUSION

A MRT version of the LB kinetic model for combustion is presented. The chemical energy released in the progress of combustion is dynamically coupled into the physical system by adding a chemical term to the LB kinetic equation. The chemical term describes the change rate of distribution function $f$ due to the local chemical reaction. The LB model is required
to recover the Navier-Stokes equations with chemical reaction in the hydrodynamic limit. To that aim, the discrete equilibrium distribution function \( f_i^{eq} \) needs to satisfy 24 independent moment relations. We present a new discrete velocity model with 24 velocities which are divided into 3 groups. In each group a flexible parameter \( (v_a, v_b \text{ or } v_c) \) is used to control the size of discrete velocities and a second parameter \( (\eta_a, \eta_b \text{ or } \eta_c) \) is used to describe the contribution of the extra degrees of freedom. The current model works for both subsonic and supersonic flows with or without chemical reaction. Besides the verification and validation via well-known benchmark tests, the kinetic nature of the LB model is applied in probing the nonequilibrium effects in the system.

Compared with our previous MRT-LB model for high speed flows \[74\], the new model can be used to simulate systems with chemical reactions. The rate equation for the chemical reaction can be adjusted according to specific situations. Compared with the LB model in our previous work \[78\], where 33 discrete velocities are used and both the specific-heat ratio and the Prandtl number are fixed, the new model uses only 24 discrete velocities and both the specific-heat ratio and the Prandtl number are flexible.

The SRT-LB model can be regarded as a special case of the MRT-LB where the relaxation coefficients for various dynamic modes are the same. In the currently using version of the MRT-LB, the thermodynamic nonequilibrium effects are calculated at each simulation step. The nonequilibrium behaviors of various modes may contribute to the system evolution according to different amplification factors, while all the amplification factors becomes the same in the SRT-LB model. After considering the contribution of the extra degrees of freedom, the situation becomes more complex. Via this model we can observe the following nonequilibrium behaviors: (i) exchange of internal kinetic energy between different degrees of freedom for molecule displacements, (ii) exchange of internal kinetic energies between the displacement degrees of freedom and the internal degrees of freedom of the molecules, (iii) “overshoot” phenomena in the re-approaching equilibrium procedure becomes more significant with increasing the viscosity.

As for probing the nonequilibrium behaviors around the detonation wave in one-dimensional detonation procedure, two sets of simulation results are shown. In the first set, three sets of spacial and temporal steps are used to validate the numerical results where the physical viscosity, instead of the numerical viscosity, dominates. In the second set, three sets of collision parameters are used to study the viscosity effects. It is shown that, around
the detonation wave there is competition between the viscous effect, thermal diffusion effect and the gradient effects of physical quantities. Consequently, with decreasing collision parameters, (i) both the viscosity and the heat conductivity increase; (ii) the nonequilibrium region becomes wider and the gradients of physical quantities decrease; (iii) the position where the internal energy in the shocking degree of freedom equals the one averaged over all degrees of freedom moves away from the position for the von Neumann peak.

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