A multi-component discrete Boltzmann model for nonequilibrium reactive flows

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Abstract

We propose a multi-component discrete Boltzmann model (DBM) for premixed, nonpremixed, or partially premixed nonequilibrium reactive flows. This model is suitable for both subsonic and supersonic flows with or without chemical reaction and/or external force. A two-dimensional sixteen-velocity model is constructed for the DBM. In the hydrodynamic limit, the DBM recovers the modified Navier-Stokes equations for reacting species in a force field. Compared to standard lattice Boltzmann models, the DBM presents not only more accurate hydrodynamic quantities, but also detailed nonequilibrium effects that are essential yet long-neglected by traditional fluid dynamics. Apart from nonequilibrium terms (viscous stress and heat flux) in conventional models, specific hydrodynamic and thermodynamic nonequilibrium quantities (high order kinetic moments and their departure from equilibrium) are dynamically obtained from the DBM in a straightforward way. Due to its generality, the developed methodology is applicable to a wide range of phenomena across many energy technologies, emissions reduction, environmental protection, mining accident prevention, chemical and process industry.

Introduction

Reactive flows are ubiquitous in nature and paramount to the sustainable development of society and ecological environment all over the world. For example, chemical energy released from fossil fuel in combustion comprises over 80% the world’s energy utilization [1]. As the main human’s threats, atmospheric pollution, climate change and global warming are directly relevant to harmful emissions from reactive flows, which involve a broad range of physicochemical phenomena, interacting over various spatial and temporal scales [2]. Besides, understanding of reactive flows is helpful to prevent fires in buildings, gas explosion in mines, burst in chemical factories, etc. Due to their significant importance to human society, reactive flows have attracted considerable attention in experimental, theoretical, and numerical fields. Actually, it is a challenging issue for traditional macroscopic or microscopic models to efficiently and accurately describe combustion phenomena where the span of spatial-temporal scales is relatively large and nonequilibrium phenomena play essential roles [3, 4, 5]. In fact, the nonequilibrium effects always change physical quantities (such as density, velocity, temperature, etc) in the evolution of fluid systems away from equilibrium, especially in transient and/or extreme conditions. A promising way to address this issue is to employ a mesoscopic kinetic model, lattice Boltzmann model (LBM), based on suitably simplified versions of the Boltzmann equation [6, 7, 8, 9, 10, 11, 12, 13, 14].

Recently, LBM has emerged as a versatile tool to simulate various complex systems, including reactive flows [15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31]. Previous LBMs were successfully employed as solvers of macroscopic governing equations, such as hydro-chemical equations for incompressible systems with low Mach number [15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31]. Physical quantities (such as pressure, velocity, temperature) can be described separately by several distribution functions in traditional LBMs, which are different from the Boltzmann equation where a single distribution function contains all information. For traditional LBMs, only a few low order kinetic moments of discrete equilibrium
function are used, and the high order moments are not correctly reproduced [32]. This limitation results in the failure of recovering the complete Navier-Stokes (NS) equations and providing more information on nonequilibrium behaviours. To overcome those problems, one promising method is to resort to a variant of traditional LBM, discrete Boltzmann model (DBM), where a required number of high order moments are satisfied [33, 34, 35, 36, 37, 38]. Different from traditional LBMs, DBM contains both equilibrium and nonequilibrium physical quantities that stem from the same discrete distribution function [33, 34, 35, 36, 37, 38].

Over the past years, the versatile DBM has been effectively applied to thermal phase separation, fluid instabilities, reactive flows, etc. [33, 34, 35, 36, 37, 38]. The DBM for reactive flows was firstly presented by Yan et al. in 2013 [35]. Then, Lin et al. extended the DBM to reactive flows in a polar coordinate [36]. In 2015, Xu et al. proposed a multiple-relaxation-time DBM for reactive flows where the specific heat ratio and Prandtl number are adjustable [37]. The next year, a DBM is formulated for reactive flows where chemical reactant and product are described by two coupled distribution functions [38]. However, previous DBMs are suitable for premixed reactive flows, but not for nonpremixed or partially premixed reactive flows [35, 36, 37, 38]. For the sake of simulating both subsonic and supersonic nonequilibrium reactive flows with premixed, nonpremixed, or partially premixed reactants, we propose a multi-component DBM in this work. The DBM presents two ways to access the thermodynamic nonequilibrium behaviours. One is to measure the viscous stress and heat flux that are described by traditional NS models; The other is to calculate the kinetic moments of the difference between equilibrium and nonequilibrium discrete distribution functions, which is beyond conventional hydrodynamic models. Such capability is the main object of the present work.

**Discrete Boltzmann model**

Without loss of generality, we consider the oxidation of propane in air using the one-step overall reaction,

\[
C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O,
\]

where \(C_3H_8\), \(O_2\), \(CO_2\), and \(H_2O\) denote propane, oxygen, carbon dioxide, and water, respectively. The stoichiometric coefficients for them are \([a_{C_3H_8}, a_{O_2}, a_{CO_2}, a_{H_2O}] = [-1, -5, 3, 4]\). Nitrogen is assumed to be inert. The overall reaction rate reads

\[
\omega_{ov} = k_{ov} n_{C_3H_8} n_{O_2} \exp\left(-\frac{E_a}{RT}\right),
\]

with \(k_{ov}\) the reaction coefficient, \(n^\sigma\) molar concentration, \(E_a\) effective activation energy, \(R\) universal gas constant, \(T\) temperature. The mass change rate of species \(\sigma\) is \(\omega^\sigma = a^\sigma \cdot M^\sigma \cdot \omega_{ov}\). In addition to the one-step reaction, detailed or reduced multi-step chemical kinetics, can also be employed.

Let us introduce the discrete Boltzmann equation,

\[
\frac{\partial f_i^\sigma}{\partial t} + v_i^\sigma \cdot \nabla f_i^\sigma = \Omega_i^\sigma + R_i^\sigma + G_i^\sigma,
\]
with
\[
\Omega_T^\sigma = -\frac{1}{\tau_T} [f_T^\sigma - f_i^{\sigma eq} (n^\sigma, u, T)],
\]
\[
R_T^\sigma = \frac{1}{\tau_T} [f_T^{\sigma eq} (n^\sigma, u, T^\sigma) - f_i^{\sigma eq} (n^\sigma, u, T)],
\]
\[
G_T^\sigma = \frac{1}{\tau_T} [f_T^{\sigma eq} (n^\sigma, u^{1\sigma}, T^{1\sigma}) - f_i^{\sigma eq} (n^\sigma, u^{1\sigma}, T^{1\sigma})].
\]
Here \( f_T^\sigma \) (\( f_i^{\sigma eq} \)) indicates the discrete (equilibrium) distribution function, \( v^\sigma_i \) the discrete velocity, \( t \) (\( \tau^\sigma \)) the (relaxation) time. \( \Omega_T^\sigma \), \( R_T^\sigma \), and \( G_T^\sigma \) are the collision, reaction and force terms accounting for the molecular collision, chemical reaction and external force, respectively. The collision term in Eq. (4) obeys the conservation of mass, momentum, and energy, from which the relations between the physical quantities (\( n^\sigma, n, u^{\sigma}, u, T^\sigma, T \)) and the distribution function \( f_T^\sigma \) are obtained [33]. The symbols with (without) superscript \( \sigma \) denote the physical quantities of the species (mixture). In Eq. (5), \( n^\sigma \) and \( T^\sigma \) (\( n \) and \( T \)) denote the molar concentration and temperature after (before) chemical reaction within time step \( \tau^\sigma \). Similarly, in Eq. (6), the hydrodynamic velocity changes from \( u^\sigma \) to \( u^{\sigma} \) within time \( \tau^\sigma \) due to external force, meanwhile the temperature changes from \( T^\sigma \) to \( T^{\sigma} \). The discrete equilibrium function \( f_i^{\sigma eq} \) is linked with the formula,
\[
f^{\sigma eq} = n^\sigma \left( \frac{m^\sigma}{2\pi T} \right)^{D/2} \left( \frac{m^\sigma}{2\pi I^\sigma T} \right)^{1/2} \exp \left[ -\frac{m^\sigma (v - u)^2}{2T} - \frac{m^\sigma \eta^2}{2I^\sigma T} \right],
\] (7)
in the way that a required number of kinetic moments calculated by the integral of \( f^{\sigma eq} \) are equivalent to those by the summation of \( f_i^{\sigma eq} \). In Eq. (7), \( m^\sigma \) stands for molar mass, \( D = 2 \) space dimension, \( I^\sigma \) extra degrees of freedom corresponding to molecular rotation or vibration. There are 7 moments satisfied by \( f_i^{\sigma eq} = f_i^{\sigma eq} (n^\sigma, u, T) \) in this work. Specifically,
\[
n^\sigma = \sum_i f_i^{\sigma eq},
\]
\[
n^\sigma u = \sum_i f_i^{\sigma eq} v^\sigma_i,
\]
\[
n^\sigma \left( (D + I^\sigma) \frac{T}{m^\sigma} + u \cdot u \right) = \sum_i f_i^{\sigma eq} \left( v^\sigma_i \cdot v^\sigma_i + \eta_i^{\sigma 2} \right),
\]
\[
n^\sigma \left( \delta_{\alpha\beta} \frac{T}{m^\sigma} e_\alpha e_\beta + uu \right) = \sum_i f_i^{\sigma eq} v^\sigma_i v^\sigma_i,
\]
\[
n^\sigma u \left( (D + I^\sigma + 2) \frac{T}{m^\sigma} + u \cdot u \right) = \sum_i f_i^{\sigma eq} \left( v^\sigma_i \cdot v^\sigma_i + \eta_i^{\sigma 2} \right) v^\sigma_i,
\]
\[
n^\sigma \left( u_\alpha e_\beta e_\chi \delta_{\beta\chi} + e_\alpha u_\beta e_\chi \delta_{\beta\chi} + e_\alpha e_\beta u_\chi \delta_{\alpha\beta} \right) \frac{T^\sigma}{m^\sigma} + n^\sigma uu = \sum_i f_i^{\sigma eq} v^\sigma_i v^\sigma_i v^\sigma_i,
\]
\[
n^\sigma \delta_{\alpha\beta} e_\alpha e_\beta \left( (D + I^\sigma + 2) \frac{T}{m^\sigma} + u \cdot u \right) \frac{T}{m^\sigma} + n^\sigma uu \left( (D + I^\sigma + 4) \frac{T}{m^\sigma} + u \cdot u \right)
\]
\[
= \sum_i f_i^{\sigma eq} \left( v^\sigma_i \cdot v^\sigma_i + \eta_i^{\sigma 2} \right) v^\sigma_i v^\sigma_i,
\]
which can be expressed in an uniform form \( \hat{f}^{\sigma eq} = M f^{\sigma eq} \), where
\[
\hat{f}^{\sigma eq} = \left( f_1^{\sigma eq}, f_2^{\sigma eq}, \ldots, f_{N_1}^{\sigma eq} \right)^T,
\]
\[
M = \left( \begin{array}{cccc}
M_{11} & M_{12} & \cdots & M_{1N_1} \\
M_{21} & M_{22} & \cdots & M_{2N_1} \\
\vdots & \vdots & \ddots & \vdots \\
M_{N_1,1} & \vdots & \cdots & M_{N_1,N_1}
\end{array} \right),
\]
with \( N_1 = 16 \). The elements of \( \hat{f}^{\sigma eq} \) are \( \hat{f}_1^{\sigma eq} = n^\sigma, \hat{f}_2^{\sigma eq} = n^\sigma u_\alpha, \hat{f}_3^{\sigma eq} = n^\sigma u_\alpha u_\beta, \hat{f}_4^{\sigma eq} = n^\sigma u_\alpha u_\beta u_\gamma, \hat{f}_5^{\sigma eq} = n^\sigma (T/m^\sigma + u_\beta^2), \hat{f}_6^{\sigma eq} = n^\sigma u_\alpha u_\beta u_\gamma, \hat{f}_7^{\sigma eq} = n^\sigma (T/m^\sigma + u_\beta^2), \hat{f}_8^{\sigma eq} = n^\sigma u_\alpha u_\beta u_\gamma, \hat{f}_9^{\sigma eq} = n^\sigma u_\alpha u_\beta u_\gamma (D + I^\sigma + 2)T/m^\sigma + u_\beta^2, \hat{f}_{10}^{\sigma eq} = 3n^\sigma u_\alpha u_\beta T/m^\sigma + n^\sigma u_\beta^2, \hat{f}_{11}^{\sigma eq} = n^\sigma u_\alpha u_\beta T/m^\sigma + n^\sigma u_\beta^2 u_\gamma, \hat{f}_{12}^{\sigma eq} = n^\sigma u_\alpha u_\beta T/m^\sigma + n^\sigma u_\beta^2 u_\gamma (D + I^\sigma + 2)T/m^\sigma + u_\beta^2, \hat{f}_{13}^{\sigma eq} = 3n^\sigma u_\alpha u_\beta T/m^\sigma + n^\sigma u_\beta^2 u_\gamma, \hat{f}_{14}^{\sigma eq} = n^\sigma ((D + I^\sigma + 2)T/m^\sigma + u_\beta^2)T/m^\sigma + n^\sigma u_\beta^2 (D + I^\sigma + 4)T/m^\sigma + u_\gamma^2, \hat{f}_{15}^{\sigma eq} = n^\sigma u_\alpha u_\beta u_\gamma (D + I^\sigma + 4)T/m^\sigma + u_\gamma^2, \hat{f}_{16}^{\sigma eq} = n^\sigma ((D + I^\sigma + 2)T/m^\sigma + u_\beta^2)T/m^\sigma + n^\sigma u_\beta^2 (D + I^\sigma + 4)T/m^\sigma + u_\gamma^2, \end{align*}
and those of M are $M^0 = 1$, $M^1_x = v^0_{xx}$, $M^2_y = v^0_{xx}$, $M^3_y = v^0_{xx} + \eta^2$, $M^4_{xx} = v^0_{xx} + \eta^2$, $M_{xx} = v^0_{xx}$, $M_{xx} = (v^0_{xx} + \eta^2)v^2_{xx}$, $M_{xx} = (v^0_{xx} + \eta^2)v^2_{xx}$, $M_{xx} = (v^0_{xx} + \eta^2)v^2_{xx}$, $M_{xx} = (v^0_{xx} + \eta^2)v^2_{xx}$.

The discrete velocities $v^\sigma$ and $\eta^\sigma$ are (see Fig. [4]),

$$[v^\sigma, \eta^\sigma] = \begin{cases} 
[cyc: v^\sigma (\pm 1, 0), \eta^\sigma] & 1 \leq i \leq 4, \\
[cyc: v^\sigma (\pm 1, \pm 1), \eta^\sigma] & 5 \leq i \leq 8, \\
[cyc: v^\sigma (\pm 1, 0), \eta^\sigma] & 9 \leq i \leq 12, \\
[cyc: v_i^\sigma (\pm 1, \pm 1), \eta^\sigma] & 13 \leq i \leq 16,
\end{cases} \quad (15)$$

where cyc indicates the cyclic permutation, $(v^\sigma, v^\sigma, v^\sigma, v^\sigma, v^\sigma, v^\sigma, v^\sigma, v^\sigma)$ are adjustable parameters. And the discrete equilibrium distribution is expressed by

$$f^{eq} = M^{-1} f^{eq}.$$ 

One significant capability of the DBM is to investigate nonequilibrium manifestations by measuring the following physical variables,

$$\Delta^2_\sigma = \sum_i m^\sigma (f_i^\sigma - f_i^{eq\sigma}) v_i^\sigma v_i^\sigma, \quad (17)$$

$$\Delta^2_{\alpha, \beta} = \sum_i m^\sigma (f_i^\sigma - f_i^{eq\sigma}) (v_i^\sigma \cdot v_i^\sigma + \eta_i^\sigma v_i^\sigma), \quad (18)$$

$$\Delta^2_\sigma = \sum_i m^\sigma (f_i^\sigma - f_i^{eq\sigma}) v_i^\sigma v_i^\sigma, \quad (19)$$

$$\Delta^2_{\alpha, \beta} = \sum_i m^\sigma (f_i^\sigma - f_i^{eq\sigma}) (v_i^\sigma \cdot v_i^\sigma + \eta_i^\sigma v_i^\sigma). \quad (20)$$

Mathematically, $\Delta^2_\sigma = \Delta^2_{2\alpha, \beta} + \delta_{\sigma} \delta_{\sigma} e_{\sigma} e_{\sigma}$ is a second order tensor with four components, among which only three ($\Delta^2_{xx}, \Delta^2_{xy}, \Delta^2_{yy}$) are independent; $\Delta^2_{3\alpha, \beta} = \Delta^2_{3\alpha, \beta} e_{\sigma} e_{\sigma} e_{\sigma}$ is a third order tensor with eight components where only four ($\Delta^2_{3xx}, \Delta^2_{3xy}, \Delta^2_{3yy}, \Delta^2_{3yxy}$) are independent; $\Delta^2_{4, 1} = \Delta^2_{4, 1} e_{\sigma}$ is the first order tensor (i.e. vector) contracted from a third order tensor and have two components; Similarly for $\Delta^2_{4, 2} = \Delta^2_{4, 2} e_{\sigma} e_{\sigma}$.

It is easy to prove that, via the Chapman-Enskog multiscale analysis, the DBM is in line with the following modified NS equations,

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial \chi} (\rho^2 u_{\alpha}) = \rho \sigma, \quad (21)$$

$$\frac{\partial}{\partial t} (\rho^2 u_{\alpha}) + \frac{\partial}{\partial \chi} \left( \rho^2 u_{\alpha} u_{\beta} + \Delta^{2}_{\alpha, \beta} \right) = \rho^2 a_{\alpha} - \frac{\rho^2}{\tau} (u_{\alpha} - u_{\alpha}) + \rho \sigma \cdot u_{\alpha}, \quad (22)$$

$$\frac{\partial}{\partial t} \sigma = \frac{\partial}{\partial \chi} \left( \frac{\rho^2 u_{\alpha} u_{\alpha} + \Delta^{2}_{\alpha, \beta} \rho \sigma}{\rho^2} \right) + \rho \sigma \cdot \left( \frac{D + I^2}{2m^\sigma} I + \frac{1}{2} u^2 \right) + \frac{D + I^2}{2m^\sigma} \rho \sigma T^2 - \rho \sigma \left( \frac{D + I^2 + 2}{2m^\sigma} \rho \sigma \right) \cdot \left( \frac{D + I^2}{2m^\sigma} + \rho \sigma \right) - \frac{\rho^2}{\tau} \left( \frac{D + I^2}{2m^\sigma} + \rho \sigma \right)^2, \quad (23)$$

in the hydrodynamic limit, with $\Delta^{2}_{\alpha, \beta} = P_{\alpha, \beta} + U_{\alpha, \beta}$, $\Delta^{2}_{\alpha, \beta} = -\kappa_{\alpha, \beta} \sigma / \rho^2 + \partial / \rho^2 - \frac{\partial}{\rho^2} \frac{\partial}{\rho^2}$, $U_{\alpha, \beta} = \rho/\rho^2 (\rho^2 + \rho^2 + \rho^2) (\rho^2 - \rho^2 + \rho^2) ^2$, $\rho^2 = (D + I^2)^2 / (2m^\sigma)$ internal energy per unit mass, $\rho^2 = \rho/\rho^2 (\rho^2 + \rho^2 + \rho^2)$ normal dynamic viscosity coefficient, $\sigma = \gamma^\sigma \mu^\sigma$ heat conductivity, and $\gamma^\sigma = (D + I^2) / (2m^\sigma)$ specific heat ratio. The superscript "cyc" represents the change rate of physical quantities due to the chemical reaction. In fact, applying the operator $\sum_{\sigma}$ to both sides of Eqs. (21) - (23) gives NS equations for the whole system, which reduces to conventional NS equations when $u^\sigma = u$ and $T^\sigma = T$. Obviously, Eqs. (21) - (23) gives a more detailed description than the conventional NS equations. The latter is just a special case of the former.

Furthermore, dynamic viscosity and heat conductivity in the NS equations are regarded as two important thermodynamic nonequilibrium manifestations or physical effects on fluid flows. In fact, a more detailed way to study the nonequilibrium behaviours is to investigate the departure of high order velocity moments from their local equilibrium counterparts, as shown in Eqs. (17) - (20). Those kinetic moments of the difference between nonequilibrium and equilibrium distribution functions have significant physical meanings. In particular, $\Delta^{2}_{\sigma}$ is associated with viscous stress tensor and nonorganised momentum fluxes, $\Delta^{2}_{\sigma}$ and $\Delta^{2}_{\sigma}$ are related to nonorganised energy (heat) fluxes, $\Delta^{2}_{\sigma, 2}$ corresponds to the flux of nonorganised energy (heat) flux [36, 37]. The terminology "nonorganised" is relative to "organised". The latter refers to the collective motion of a fluid flow, while the former corresponds to the molecular individualism on top of the collective motion [31]. Moreover, $1/2 m_{\sigma} \sigma (f^{eq\sigma}) = 1/2 \sum_{i} m^\sigma f_{x_i}^x v_{x_i}^2$ is defined as the translational energy of species $\sigma$ in $\alpha$ direction, $1/2 m_{\sigma} \sigma (f^{eq\sigma})$ is
its equilibrium counterpart, and \( \frac{1}{2} \Delta \sigma_{2\alpha}^{\alpha} = \frac{1}{2} \text{H}_{2\alpha}(f^{\alpha}) - \frac{1}{2} \text{H}_{2\alpha}(f^{\sigma eq}) \) the nonorganised energy of species \( \sigma \) in \( \alpha \) direction; \( \frac{1}{2} \text{H}_{3,1\alpha}(f^{\sigma eq}) = \frac{1}{2} \sum_i m_i \sigma^2_i (v_i^{\sigma eq} + \eta_i^2) v_i^\alpha \) refers to the organised flux of energy in \( \alpha \) direction, \( \frac{1}{2} \Delta \sigma_{3,1\alpha}^{\alpha} \) the nonorganised flux of energy in \( \alpha \) direction, and \( \frac{1}{2} \text{H}_{3,1\alpha}(f^{\sigma}) = \frac{1}{2} \text{H}_{3,1\alpha}(f^{\sigma eq}) + \frac{1}{2} \Delta \sigma_{3,1\alpha}^{\alpha} \) the total flux of energy in \( \alpha \) direction. Obviously, DBM provides more nonequilibrium information on various species in fluid flows, which is an essential advantage over traditional models.

**Numerical simulation**

To validate this DBM, we conduct five simulation tests. Test one is the combustion of (premixed, nonpremixed, and partially premixed) propane-air filled in a free-falling box. The released heat in constant volume and the external force effects are demonstrated. The second test is a subsonic flame at constant pressure. In the third part, to show its suitability for high-speed compressible systems, the DBM is used to simulate a shock wave. Its capability to investigate nonequilibrium effects is verified as well. A supersonic reacting wave is simulated in the fourth part. The first four tests are 1-dimensional (1-D) cases. The last is for a typical 2-D case, Kelvin-Helmholtz (KH) instability.

Moreover, the first order Euler forward time discretization and the second order nonoscillatory and nonfree-parameters dissipative finite difference scheme \( [59] \) are adopted for the temporal and spatial derivatives in Eqs. \( [3] - [10] \) in this section. Hence, the discrete velocities \( v_i \) are independent of the grid mesh \( \Delta x \) and \( \Delta y \). For the purpose of accuracy and robustness, it is preferable to set the values of discrete velocities \( \{v_i^\sigma, v_i^\alpha, v_i^{\sigma eq}, v_i^\sigma e\} \) around the values of \( |u| \) and \( \sqrt{DT/m^2} \), and choose \( \{\eta_i^\sigma, \eta_i^\alpha, \eta_i^{\sigma eq}, \eta_i^\sigma e\} \) around the value \( \sqrt{I^2{T}/m^2} \), which is reasonable on account of Eqs. \( [3] - [10] \).

**Combustion in constant volume**

First of all, we simulate the combustion of propane-air filled in a free-falling box, which consists of three parts with volumes \( V_1, V_2 \) and \( V_3 \), respectively. The fixed volume of the box is \( V_0 = V_1 + V_2 + V_3 \), and \( V_1 : V_2 : V_3 = 3 : 119 : 78 \). Initially, the left part is filled with propane, the middle part is full of air, and the right part is occupied by the propane-air mixture with equivalence ratio \( 0.6 \). In each part, the particle number density is \( 40.6 \text{mol}\cdot\text{m}^{-3} \), temperature \( 300 \text{K} \), and pressure \( 1 \text{atm} \). Premixed, nonpremixed and partially premixed combustion phenomena take place simultaneously in this box after ignition. Specifically, the nonpremixed combustion takes place between the left and middle parts, the partially premixed combustion occurs between the middle and right parts with a changing equivalence ratio, and the premixed combustion is in the rightmost part with a constant equivalence ratio. Three discrete velocity models (D2V16, D2V24 \( [57] \), and D2V65 \( [40] \) are employed for this simulation. The grid is \( N_x \times N_y = 200 \times 1 \), spatial step \( \Delta x = \Delta y = 5 \times 10^{-7} \text{m} \), temporal step \( \Delta x = \Delta y = 1.25 \times 10^{-10} \text{s} \).

Figure 2 illustrates the simulation results and exact solutions during the chemical reaction in the free-falling box. Theoretically, the density remains constant, \( \rho = 1.30290 \text{kg} \cdot \text{m}^{-3} \), the velocity changes as \( u_y = g t \) with \( g = -9.8 \text{m}\cdot\text{s}^{-2} \), and the sum of internal energy and chemical heat remains constant, \( E = 2.59050 \times 10^6 \text{J} \cdot \text{m}^{-3} \). As for the simulation, each model (D2V16, D2V24 \( [57] \), and D2V65 \( [40] \)) gives the density \( \rho = 1.30290 \text{kg} \cdot \text{m}^{-3} \) and the energy \( E = 2.59050 \times 10^6 \text{J} \cdot \text{m}^{-3} \) in the whole process, which coincide with the exact solutions. There are tiny differences between the simulation results and exact solutions of the velocity. For example, at time \( t = 3 \times 10^{-4} \text{s} \), the three models (D2V16, D2V24 \( [57] \), and D2V65 \( [40] \)) give simulation results \( u_y = -2.9402 \times 10^{-3}, -2.9399 \times 10^{-3}, \) and \(-2.9401 \times 10^{-3} \text{m} \cdot \text{s}^{-1} \), respectively. Compared to the exact value \( u_y = -2.94 \times 10^{-3} \text{m} \cdot \text{s}^{-1} \),
Their relative errors are 0.0068%, 0.0034%, and 0.0034%, respectively. Obviously, all simulation results agree well with the exact solutions.

Furthermore, after the chemical reaction is completed, the adiabatic constant volume temperature is 2078 K calculated by the three DBMs, while it is 2614 K obtained by the standard LBM [12, 41]. The parameters for the LBM in this work are the same as those in Ref. [41]. Compared with the experimental datum 2080 K [42], the relative differences are 0.1% for the DBM and 25.7% for the standard LBM, respectively. Physically, the DBM is suitable for compressible systems with adjustable ratio of specific heats, while the LBM in Refs. [12, 41] can only be used for the case with constant pressure and fixed ratio of specific heats.

To discuss computational costs of various discrete velocity models, we keep a record of computing times required by the aforementioned simulation in Table 1. The computational facility is a personal computer with Intel(R) Core(TM) i7-6700K CPU @ 4.00GHz and RAM 32.00 GB. There are 16, 24, and 65 (16, 24, and 16) discrete velocities (moment relations) in D2V16, D2V24 [37], and D2V65 [40], respectively. And the computing times are 1560 s, 3960 s, and 4980 s for the three models, respectively. Obviously, D2V24 and D2V65 models need larger RAM and longer time than D2V16 model.

Table 1: Computing times for simulation of combustion in constant volume with various models.

| Model | Number of discrete velocities | Number of moment relations | Computing time |
|-------|------------------------------|----------------------------|---------------|
| D2V16 | 16                           | 16                         | 1560 s        |
| D2V24 | 24                           | 24                         | 3960 s        |
| D2V65 | 65                           | 16                         | 4980 s        |

Flame at constant pressure

Let us simulate a flame at constant pressure. It travels with subsonic speed in a channel from left to right. In front of the flame is the propane-air mixture with equivalence ratio 0.6, particle number density 44.6 mol·m⁻³, temperature 300 K, and pressure 1 atm. The grid is \( N_x \times N_y = 2500 \times 1 \), spatial step \( \Delta x = \Delta y = 2 \times 10^{-5} \) m, temporal step \( \Delta t = 1.25 \times 10^{-10} \) s.

Figure 3 shows the evolution of \( \omega_{ov} \) (left) and \( \Delta_{2xx}^0 \) (right) versus \( x \). The peak of \( \omega_{ov} \) corresponding to the most active chemical reaction is ahead of the trough of \( \Delta_{2xx}^0 \), where nonequilibrium manifestations are intense and physical gradients are sharp. Note that the nonequilibrium manifestations can be employed to capture the flame or other interfaces [34]. The flame speed, 0.71 m/s, can be obtained from the profiles of either \( \omega_{ov} \) or \( \Delta_{2xx}^0 \). And the flow velocity is 0.60 m/s in front of the flame. Hence, the burning velocity is \( (0.71 - 0.60) \text{m/s} = 0.11 \text{m/s} \), which equals the experimental result 0.11 m/s [43]. While the standard LBM [41] gives a relative error, 9.1%, compared with the experimental result [44].

Moreover, in the DBM simulation, the pressure is close to 1 atm around the flame, and the temperature is 1705 K behind the flame, which is consistent with the experiment [2], while the temperature is 2028 K in the traditional LBM [12, 41] (see Fig. 4). The latter’s relative error is 18.9% compared with the experimental result [2]. Physically, the ratio of specific heats in the DBM is tunable, while the one in the LBM in Refs. [12, 41] is fixed at 2. Besides, the chemical reaction does not affect the flow field in this LBM [41], while the chemical reaction and fluid flow are naturally coupled in our DBM.
Shock wave

A shock wave is a type of disturbance that propagates faster than the local speed of sound in a fluid with significant compressible effects. Its applications cover the fields of medicine, astrophysics, industrial engineering, etc. For example, it becomes effective medical treatment for kidney and ureteral stones. It can be used for cell transformation, preservative impregnation in bamboo, sandal oil extraction, and removal of micron size dust from silicon wafer surfaces [44]. To validate the DBM for high-speed compressible systems, we conduct the simulation of a shock wave. The wave propagates in the air from left \( L \) to right \( R \). The initial field is,

\[
\begin{align*}
(\rho, u_x, u_y, T)_L &= (1.58407 \text{kg} \cdot \text{m}^{-3}, 106.637 \text{m} \cdot \text{s}^{-1}, 0 \text{m} \cdot \text{s}^{-1}, 333.612 \text{K}) \\
(\rho, u_x, u_y, T)_R &= (1.17092 \text{kg} \cdot \text{m}^{-3}, 0 \text{m} \cdot \text{s}^{-1}, 0 \text{m} \cdot \text{s}^{-1}, 300 \text{K})
\end{align*}
\]

(24)

The grid is \( N_x \times N_y = 40000 \times 1 \), spatial step \( \Delta x = \Delta y = 1 \times 10^{-8} \text{m} \), temporal step \( \Delta t = 1.25 \times 10^{-12} \text{s} \). Figure 5 plots the profiles of the shock: (a) \( \rho \), (b) \( u_x \), (c) \( T \), (d) \( p \). The squares denote DBM results, the lines exact solutions. The DBM results behind the shock wave are \( (\rho, u_x, u_y, T) = (1.58407 \text{kg} \cdot \text{m}^{-3}, 106.637 \text{m} \cdot \text{s}^{-1}, 0 \text{m} \cdot \text{s}^{-1}, 333.612 \text{K}) \), which equal the exact values in Eq. (24) precisely.

To exhibit the capability of the DBM to study nonequilibrium behaviours, Fig. 6 shows the nonequilibrium manifestations around the shock wave. Figure 6(a) displays the translational energy of oxygen in \( x \) direction \( \frac{1}{2} M^{O_2}_{2xx} (f) \), its equilibrium counterpart \( \frac{1}{2} M^{O_2}_{2xx} (f^{eq}) \), and the exact solution \( n^{O_2} T + \rho^{O_2} u_x^2 \). Figure 6(b) illustrates...
Figure 6: Nonequilibrium manifestations around the shock wave: (a) translational energy of oxygen in $x$ direction, (b) departure of translational energy of oxygen in $x$ direction from equilibrium state, (c) translational energy of nitrogen in $x$ direction, (d) departure of translational energy of nitrogen in $x$ direction from equilibrium state.

the departure of translational energy of oxygen in $x$ degree of freedom from its equilibrium state $\frac{1}{2} \Delta O_{2x}$. Figures 6 (c) and (d) are for nitrogen. It is clear that $M_{2x}^0 (f^{eq})$ coincides with the solution $n T + \rho u_x^2$ in panels (a) and (c), respectively. Physically, the translational energy of oxygen (or nitrogen) in $x$ degree of freedom travels faster than its equilibrium counterpart. Consequently, its departure from the equilibrium state is greater than zero around the shock wave. Furthermore, there are few differences between the DBM and the approximate solution [38] in panels (b) and (d), respectively. Because the approximate solution is obtained by the first-order truncation of distribution function [38]. The simulation results are satisfactory.

The grid is $N_x \times N_y = 8000 \times 1$, spatial step $\Delta x = \Delta y = 5 \times 10^{-7}$ m, temporal step $\Delta t = 6.25 \times 10^{-11}$ s.

Figure 7 displays the wave profiles: (a) $\rho$, (b) $u_x$, (c) $T$, (d) $p$. The squares indicate DBM results, the lines analytic solutions of Zeldovich-Neumann-Doering (ZND) theory [2]. The DBM results behind the wave are $(\rho, u_x, u_y, T) = (2.00166 \text{kg} \cdot \text{m}^{-3}, 666.352 \text{m} \cdot \text{s}^{-1}, 0 \text{m} \cdot \text{s}^{-1}, 2363.81 \text{K})$. Compared with the first row in Eq. (25), the relative differences are 0%, 0%, 0%, and 0.8%, respectively. Moreover, DBM gives the wave speed $1632 \text{m/s}$, and the analytic solution is $1631.6 \text{m/s}$. The relative difference between them is 0.02%. Additionally, there are slight differences between the theoretical and numerical results around the wave peak. Physically, the ZND theory assumes a sharp discontinuity at the wave peak and ignores the viscosity, heat conduction and other nonequilibrium effects [2]. On the other hand, the DBM takes into account the viscosity, heat conduction and other transport processes. Thus, the DBM is more reliable than the simple ZND theory.
Figure 7: Profiles of a supersonic reacting wave: (a) mass density $\rho$, (b) velocity $u_x$, (c) temperature $T$, (d) pressure $p$. The squares stand for DBM results, the lines exact solutions.

Figure 8: The molar fraction of propane in the evolution of KH instability at various times: (a) $0$ s, (b) $5 \times 10^{-4}$ s, (c) $10^{-3}$ s, (d) $2 \times 10^{-3}$ s.

Figure 9: Pressure and velocity fields in the evolution of KH instability at time $10^{-3}$ s.
the DBM has the potential to offer more accurate information to help design devices operating in transient
currently. Since the DBM can provide detailed distributions of nonequilibrium quantities, it permits the assessment
of kinetic moments and their departure from equilibrium) can be calculated in the DBM dynamically and
heat flux) in NS models, more detailed hydrodynamic and thermodynamic nonequilibrium quantities (high
order kinetic moments). In addition to the usual nonequilibrium terms (viscous stress and
Enskog multiscale analysis, the DBM recovers the modified NS equations for reactive species with external
premixed combustion, from subsonic to supersonic fluid flows, in or out of equilibrium. Through the Chapman-
extra degrees of freedom are taken into account. This model is suitable for premixed, nonpremixed or partially
for internal energies in extra degrees of freedom. The specific heat ratio of each species
is proposed with adjustable parameters (\(\sigma\)).

We present a reactive multi-component DBM in combination with a one-step overall chemical reaction. The
models, more detailed hydrodynamic and thermodynamic nonequilibrium quantities (high
order kinetic moments and their departure from equilibrium) can be calculated in the DBM dynamically and
conveniently. Since the DBM can provide detailed distributions of nonequilibrium quantities, it permits to assess
the corresponding numerical predictions of NS models without considering the nonequilibrium effects. Hence,
the DBM has the potential to offer more accurate information to help design devices operating in transient
}

**Kelvin-Helmholtz instability**

To demonstrate that the DBM has a good ability of capturing interface deformation, we simulate a typical 2-D
phenomenon, KH instability. The initial field, with area \(0.6m \times 0.2m\), consists of two parts. The left part is full
of propane with vertical speed \(200m \cdot s^{-1}\), while the right part is filled with air with \(-200m \cdot s^{-1}\). Considering
the transition layer between the two parts, the field jump at the interface is smoothed by a tanh profile with
width \(0.002m\). The temperature is 300 K, and pressure 1 atm. Between the propane and air is a sinusoidal
interface with amplitude \(0.003m\), which is used to promote the KH instability. Moreover, the outflow and periodic
boundary conditions are adopted in the \(x\) and \(y\) directions, respectively. The grid is \(N_x \times N_y = 3000 \times 1000\),
spatial step \(\Delta x = \Delta y = 2 \times 10^{-4} m\), temporal step \(\Delta t = 2.5 \times 10^{-8} s\).

Figure 8 shows the molar fraction of propane at four different times. Initially, the interface starts to wrinkle
due to the initial perturbation and velocity shear. A rolled-up vortex emerges after the initial linear growth stage. Then there is a large vortex around the interface. The evolution of the field is qualitatively similar to previous studies [38, 45]. Moreover, Fig. 9 delineates the contour of pressure with velocity field, corresponding to Fig. 8(c). Compared Fig. 9 with Fig. 8(c), we can find that the minimum pressure, \(p = 0.257atm\), is located at, \((0.300m, 0.0750m)\), the center of the vortex. While the maximum, \(p = 1.24atm\), takes place at, \((0.3008m, 0.1708m)\), where counterflows above the vortex encounter each other and the horizontal velocity is close to zero. Physically, the pressure gradient around the vortex provides the centripetal force for the rotating flow.

To quantitatively validate the results, we plot the logarithm of absolute value of the minimum perturbed
horizontal velocity, \(\ln |u_{x-min}|\), versus time, see Fig. 10. The squares are for DBM results, the solid line
represent f the fitting function \(F(t) = -3.89713 + 11.3302t\), and the dashed line stands for the analytic solution
\(F(t) = -3.95865 + At\) with the growth rate \(A = 12.0995\) [46]. Here the nondimensionalization is used the same
as Ref. [46]. The relative difference of the growth rate between the fitting function and the analytic solution
is 6.4%. Furthermore, we compare the simulation frequency 1256 Hz with the analytic solution 1248 Hz [38, 46].
The relative difference is 0.6%. The difference mainly comes from the fact that the effects of compressibility,
viscosity, and heat conduction are considered by the DBM, but ignored by the analytic theory [46].

**Conclusions**

We present a reactive multi-component DBM in combination with a one-step overall chemical reaction. The
effects of chemical reaction and external force are considered. A two-dimensional sixteen-velocity model D2V16
is proposed with adjustable parameters (\(v^c_a, v^c_b, v^c_c, v^c_d\)) controlling discrete velocities and (\(\eta^c_a, \eta^c_b, \eta^c_c, \eta^c_d\))
for internal energies in extra degrees of freedom. The specific heat ratio of each species \(\sigma\) is flexible since
extra degrees of freedom are taken into account. This model is suitable for premixed, nonpremixed or partially
premixed combustion, from subsonic to supersonic fluid flows, in or out of equilibrium. Through the Chapman-Ensikog multiscale analysis, the DBM recovers the modified NS equations for reactive species with external
force effects in the hydrodynamic limit. In addition to the usual nonequilibrium terms (viscous stress and
heat flux) in NS models, more detailed hydrodynamic and thermodynamic nonequilibrium quantities (high
order kinetic moments and their departure from equilibrium) can be calculated in the DBM dynamically and
conveniently. Since the DBM can provide detailed distributions of nonequilibrium quantities, it permits to assess
the corresponding numerical predictions of NS models without considering the nonequilibrium effects. Hence,
the DBM has the potential to offer more accurate information to help design devices operating in transient

![Figure 10: Evolution of the velocity perturbation, \(\ln |u_{x-min}|\). The squares stand for DBM results, the solid (dashed) line is for the fitting function (analytic solution).](image-url)
and/or extreme conditions away from equilibrium. Furthermore, thanks to its mesoscopic nature, the DBM could provide deeper insight into ubiquitous reactive or nonreactive fluid flows with a large span of spatial-temporal scales. Finally, due to its generality, the developed methodology is applicable to a wide range of phenomena across many energy technologies, emissions reduction, environmental protection, mining accident prevention, chemical and process industry.

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Author contributions

S.S. contributed to the analysis of the theory and results of the DBM; L.F. provided the code of standard LBMs and assisted in performing the simulations; K.L. initiated and supervised the study; C.L. developed and validated the DBM as well as drafted the manuscript. All authors modified and approved the manuscript.

Additional information

Competing financial interests: The authors declare no competing financial interests.