Polar coordinate lattice Boltzmann kinetic modeling of detonation phenomena

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\textbf{Abstract}

A polar coordinate lattice Boltzmann kinetic model for detonation phenomena is presented and applied to investigate typical implosion and explosion processes. Main focuses are the nonequilibrium behaviors in these processes. The system at the disc center is always in its thermodynamic equilibrium. The internal kinetic energies in different degrees of freedom show the maximum difference at the inflexion point where the pressure has the largest spatial derivative. The dependence of the reaction rate on the pressure, influences of the shock strength and reaction rate on the departure amplitude of the system from its local thermodynamic equilibrium are probed.

\textit{Keywords:} Lattice Boltzmann; Combustion; Detonation; Nonequilibrium effects

\section{1. Introduction}

The rapid and violent form of combustion called detonation \textsuperscript{1} propagates through detonation wave which is a shock wave with chemical reaction. Given a wide range of application in science and engineering, shock and detonation have always been of great concern in the field of science and technology \textsuperscript{1, 2, 3}. The detonation phenomena are widely used in the acceleration of various projectiles, mining technologies, depositing of coating to a surface or cleaning of equipment, etc. Early in 1899 and 1905, Chapmann \textsuperscript{4} and Jouguet \textsuperscript{5} presented CJ theory. This theory assumes that detonation front is a strong discontinuous plane with
chemical reaction which immediately completes as soon as the detonation wave passes. In 1940s, Zeldovich [6], Neumann [7] and Doering [8] presented the well-known ZND model. This model gives an important conclusion that there is von-Neumann-peak at detonation wave front. Reactant is firstly pre-compressed by shock wave, and there is a continuous reaction zone behind the shock wave. Physical quantities (density, temperature, pressure and velocity) reach maximum values within the reaction zone.

Although detonation has been studied for more than one century [9], it remains an active area of research in both theoretical studies and numerical simulations [10] due to its practical importance [11]. So far, all chemical reaction models are empirical or semi-empirical formulas [12], such as the Arrhenius kinetics, forest fire burn, two-step model, Cochran’s rate function [13], Lee-Tarver model [14], etc. Selecting appropriate chemical reaction kinetics is very important for describing detonation phenomena under consideration. In this paper, we adopt Cochran’s rate function for chemical reaction, which is one of the most physically justifiable models satisfying simulation and experimental results [15, 16].

During recent years, Lattice Boltzmann (LB) method has achieved great success in various fields of fluid dynamics and beyond [17, 18]. LB modeling for chemical reactions or combustion phenomena [19, 20, 21, 22, 23, 24, 25] has been an interesting topic from early days. However, the progress was very limited, because previous studies on LB model were mainly focused on isothermal and incompressible fluid systems. Those models generally cannot recover the correct energy equation or describe enough the compressibility in the hydrodynamic limit, which make difficult the modeling of systems with shock and/or detonation. At the same time, most of those LB models assume that exothermic reaction has no significant effect on fluid field, which also constrains the practical application of the models to most cases of combustion. In recent years, the development of LB models for high speed compressible flows [26, 27, 28, 29, 30, 31, 32, 33] makes it possible to simulate systems with shock and detonation. Very recently Yan, Xu, Zhang, et al. proposed a Lattice Boltzmann Kinetic Model (LBKM) for detonation phenomena in Cartesian coordinates [34]. For simulating the explosion and implosion behaviors, a polar coordinate LB model is obviously more convenient. And there are many nice papers about LB formulations for axisymmetric flows in polar coordinates [35, 36, 37, 38, 39]. In 2011 Watari [40] proposed a finite-difference
LB methods in polar coordinate system. Recently we \cite{41} improved the LBKM by using a hybrid scheme so that it works also for supersonic flows. Within the improved model, the temporal evolution is calculated analytically and the convection term is solved via a Modified Warming-Beam (MWB) scheme. In this work, a new polar coordinate LBKM which is similar to and simpler than the one in Ref.\cite{41} is used to study detonation phenomena.

In contrast to traditional methods based on Navier-Stokes description, the LBKM has some intrinsic superiority in describing kinetic mechanisms in systems where equilibrium and non-equilibrium behaviors coexist \cite{18,33,34,41}. The mini-review \cite{33} presented a methodology to investigate non-equilibrium behaviors of the system by using the LB method. The non-equilibrium behaviors in various complex systems attract great attention \cite{34,41,42,43}. In the work \cite{34} by Yan, Xu, Zhang, et al., some non-equilibrium behaviors around the von Neumann peak are obtained. In a recent work \cite{41} we studied the non-equilibrium characteristics of the system around three kinds of interfaces, the shock wave, the rarefaction wave and the material interface, for two specific cases. We draw qualitative information on the actual distribution function. In this work, we further investigate the macroscopic behaviors due to deviating from local thermodynamic equilibrium in the detonation procedure.

The rest of the paper is structured as follows. In section II the polar coordinate LBKM for compressible fluid is briefly described, the treatment of inner boundary around disc center is proposed, and the manifestations of non-equilibrium characteristics are introduced. In section III we give the chemical reaction model and numerical verification, simulate implosion and explosion phenomena, and study the non-equilibrium characteristics of each case. The actual distribution functions around detonation wave are qualitatively illustrated. Section IV gives the conclusion and discussions.

2. LBKM in polar coordinates

2.1. Discrete velocity model

In a polar coordinate system, the LB equation with the Bhatanger-Gross-Krook approximation reads,

\[
\frac{\partial f_{ki}}{\partial t} + v_{kin} \frac{\partial f_{ki}}{\partial r} + \frac{1}{r} v_{kid} \frac{\partial f_{ki}}{\partial \theta} = -\frac{1}{\tau} (f_{ki} - f_{eq}^{ki}),
\]  

(1)
where $r$ ($\theta$) is the radial (azimuthal) coordinate; $f_{ki}$ ($f_{ki}^{eq}$) is the discrete (equilibrium) distribution function; $\tau$ is the relaxation time; $v_{ki\tau}$ ($v_{ki\theta}$) is the radial (azimuthal) component of the discrete velocity $v_{ki}$ as below \[40, 44],

$$v_{ki} = v_{k\tau}e_r + v_{k\theta}e_\theta, \quad v_{k\tau} = v_k \cos(i\pi/4 - \theta), \quad v_{k\theta} = v_k \sin(i\pi/4 - \theta),$$  \hspace{1cm} (2)

where $e_r$ and $e_\theta$ are unit vectors. The subscript $k$ ($= 0, 1, 2, 3, 4$) indicates the $k$-th group of the particle velocities with speed $v_k$. One speed is $v_0 = 0$, and each of the other group has 8 components. In this work we choose $v_1 = 1.5$, $v_2 = 3.5$, $v_3 = 7.5$, $v_4 = 12.5$.

In terms of local particle density $\rho$ ($= \sum_{ki} f_{ki}$), hydrodynamic velocity $u$ ($= \sum_{ki} f_{ki} v_{ki}/\rho$) and internal energy $E$ ($= \sum_{ki} \frac{1}{2} f_{ki} (v_{ki} - u) \cdot (v_{ki} - u)/\rho$), we get

$$f_{ki}^{eq} = \rho F_k [(1 - \frac{u^2}{2E} + \frac{u^4}{8E^2}) + \frac{v_{ki}\nu_\varepsilon}{E} (1 - \frac{u^2}{2E}) + \frac{v_{ki}v_{k\tau}u_\tau}{2E^2} (1 - \frac{u^2}{2E}) + \frac{v_{ki}v_{k\theta}u_\theta}{6E^3} + \frac{v_{ki\tau}v_{k\theta}u_\tau u_\theta}{24E^4}]. \hspace{1cm} (3)$$

with weighting coefficients

$$F_k = \frac{1}{v_k^2 (v_k^2 - v_{k+1}^2) (v_k^2 - v_{k-1}^2) (v_k^2 - v_{k+3}^2)} [48E^4 - 6(v_{k+1}^2 + v_{k+2}^2 + v_{k+3}^2)E^3 + (v_{k+1}^2 + v_{k+2}^2 + v_{k+3}^2)E^2 + \frac{1}{4} v_{k+1}^2 v_{k+2}^2 v_{k+3}^2],$$

$$F_0 = 1 - 8(F_1 + F_2 + F_3 + F_4),$$

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

### 2.2. LB evolution equation

The evolution equation, with first-order accuracy, used for Eq\[1\] reads

$$f_{ki}^{t+\Delta t} = f_{ki}^{eq} + (f_{ki}^{eq} - f_{ki}^{eq}) \exp(-\Delta t/\tau) + f_{ki,r}^* + f_{ki,\theta}^* \hspace{1cm} (4)$$

and

$$f_{ki,r}^* = \begin{cases} C_r [f_{ki}(i_r, i_\theta) - f_{ki}(i_r - 1, i_\theta)] & \text{for } C_r \geq 0, \\ C_r [f_{ki}(i_r + 1, i_\theta) - f_{ki}(i_r, i_\theta)] & \text{for } C_r < 0, \end{cases} \hspace{1cm} (5)$$

$$f_{ki,\theta}^* = \begin{cases} C_\theta [f_{ki}(i_r, i_\theta) - f_{ki}(i_r, i_\theta - 1)] & \text{for } C_\theta \geq 0, \\ C_\theta [f_{ki}(i_r, i_\theta + 1) - f_{ki}(i_r, i_\theta)] & \text{for } C_\theta < 0, \end{cases} \hspace{1cm} (6)$$

with Courant-numbers $C_r$ ($= v_{k\tau} \frac{\Delta t}{\Delta r}$) and $C_\theta$ ($= \frac{1}{\tau} v_{k\theta} \frac{\Delta t}{\Delta \theta}$).
2.3. Boundary conditions

The physical domain under consideration is in a sector which is only 1/8 of an annular or circular area. The azimuthal boundaries are treated with periodic boundary conditions \[41\]. For annular area with radii \(0 < R_1 < R_2\), inflow/outflow conditions are imposed at radial boundaries \[41\]. For circular area with radius \(R\), its outer radial boundary is treated in the same way. Specially, around the center, the inner boundary is treated as,

\[
f(i_r, i_\theta, k, i) = f(1 - i_r, i_\theta, k, \text{mod}(i + 4, 8)),
\]

with \(i_r = -1, 0\) for the nodes added to the computational domain and the function \(\text{mod}(a, b)\) means the remainder of \(a\) divided by \(b\). Figure 1 shows the relation between the distribution functions in the first and the fifth sector of physical domain in a periodic circular area by rotation.

2.4. Non-equilibrium characteristics

LB model naturally inherits the function of Boltzmann equation describing non-equilibrium system. The departure of the system from local thermodynamic equilibrium state can be measured by the high-order moments of \(f_{ki}\). As given in \[34, 41\], the central moments \(M_m^*\)
are defined as:

\[
\begin{align*}
M_2^*(f_{ki}) &= \sum_{ki}^{\Delta t} f_{ki} v_{ki}^* v_{ki}^* \\
M_3^*(f_{ki}) &= \sum_{ki}^{\Delta t} f_{ki} v_{ki}^* v_{ki}^* v_{ki}^* \\
M_{3,1}^*(f_{ki}) &= \sum_{ki}^{\Delta t} \frac{1}{2} f_{ki} v_{ki}^* + v_{ki} v_{ki}^* \\
M_{4,2}^*(f_{ki}) &= \sum_{ki}^{\Delta t} \frac{1}{2} f_{ki} v_{ki}^* + v_{ki} v_{ki}^* v_{ki}^* v_{ki}^* 
\end{align*}
\]

where \( v_{ki}^* = v_{ki} - u \). The manifestations of non-equilibrium are defined as:

\[
\Delta_m^* = M_m^*(f_{ki}) - M_m^*(f_{eq_{ki}}^*).
\]

In theory, \( M_3^*(f_{eq_{ki}}) = 0, M_3^*(f_{ki}) = \Delta_3^*, M_{3,1}^*(f_{eq_{ki}}) = 0, M_{3,1}^*(f_{ki}) = \Delta_{3,1}^*, M_{3,1,r}^*(f_{ki}) = \frac{1}{2}(M_{3,rrr}^*(f_{ki}) + M_{3,rr\theta}^*(f_{ki})), M_{3,1,\theta}^*(f_{ki}) = \frac{1}{2}(M_{3,rr\theta}^*(f_{ki}) + M_{3,\theta\theta}^*(f_{ki})), \Delta_{3,1,r}^*(f_{ki}) = \frac{1}{2}(\Delta_{3,rrr}^*(f_{ki}) + \Delta_{3,rr\theta}^*(f_{ki})).
\]

3. Detonation

Detonation is in a complex process with mutual influence between fluid dynamics and chemical reaction kinetics. The detonation front propagates into unburnt gas at a velocity higher than the speed of sound in front of the wave \( P \). Physical quantities at two sides of detonation front satisfy Hugoniot relations \[1\].

3.1. Chemical reaction

To describe the chemical process of detonation, we choose Cochran’s rate function presented by Cochran and Chan \[13\],

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

where \( \lambda = \rho_p/\rho \) is the mass fraction of reacted reactant, and \( \rho_p \) is the density of reacted reactant. The right side of Eq.10 is composed of a hot formation term and a growth term. \( P^m \) and \( P^n \) describe the dependence on the local pressure and \( \omega_1, \omega_2, m \) and \( n \) are adjustable parameters. Furthermore, \( T > T_{th} \) is a necessary condition for chemical reaction, with the ignition temperature \( T_{th} \). In this work, we choose \( m = n = 1, T_{th} = 1.1 \).

Via introducing the symbol, \( a = \omega_1 P^m, b = \omega_2 P^n, \lambda = \lambda_i, \lambda_{is} = \lambda_i, \lambda_{ir} = \lambda(i_r, i_\theta, t) \), the evolution of Eq.10 with first-order accuracy reads

\[
\lambda^{(i_r + \Delta t)} = \frac{(a + b\lambda)e^{(a+b)\Delta t} - a(1 - \lambda)}{(a + b\lambda)e^{(a+b)\Delta t} + a(1 - \lambda)} + \lambda_{ir}^* + \lambda_{is}^*.
\]
and

\[
\lambda^*_{ir} = \begin{cases} 
-\frac{u_r(\lambda_{ir} - \lambda_{ir-1})}{\Delta r} \Delta t & \text{for } u_r \geq 0, \\
-\frac{u_r(\lambda_{ir+1} - \lambda_{ir})}{\Delta r} \Delta t & \text{for } u_r < 0,
\end{cases}
\]

(12)

\[
\lambda^*_{i\theta} = \begin{cases} 
-\frac{u_{i\theta}(\lambda_{i\theta} - \lambda_{i\theta-1})}{r\Delta \theta} \Delta t & \text{for } u_{i\theta} \geq 0, \\
-\frac{u_{i\theta}(\lambda_{i\theta+1} - \lambda_{i\theta})}{r\Delta \theta} \Delta t & \text{for } u_{i\theta} < 0.
\end{cases}
\]

(13)

In the detonation progress, the chemical energy of reaction is transformed into heat, i.e.,

\[E^{new} = E + (\lambda^{new} - \lambda)\rho q,\]

where \(q\) is the amount of heat released by the chemical reactant per unit mass, \(\lambda\) is the parameter before local chemical reaction, \(\lambda^{new}\) is the one after local chemical reaction within one time step \(\Delta t\), \((\lambda^{new} - \lambda)\rho q\) is the released chemical energy, \(E\) is internal energy before reaction, \(E^{new}\) is the renew internal energy after reaction, meanwhile pressure \(P\) and temperature \(T\) change with the updated \(E^{new}\). Then we calculate the local equilibrium distribution function \(f_{ki}^{eq}\) from the updated physical quantities. To this step, the chemical reaction has coupled naturally with the flow behaviors by collisions.

It is worth pointing out that the Cochran’s rate function used in this work is similar to, but different from, the Lee-Tarver model used in the work [34]. The parameters \(a\) and \(b\) in Eq.11 depend on the pressure in the former work, while they are given fixed values in the latter work where the pressure plays no role in the chemical process. Consequently, the extinction phenomenon can be investigated in this work and can not be simulated in the latter work.

3.2. Simulation of steady detonation

3.2.1. Validation and verification

In this section, a steady detonation is simulated to demonstrate the validity of the new model. The initial physical quantities are as:

\[
\begin{cases} 
(p, T, u_r, u_{i\theta}, \lambda)_i = (1.35826, 2.59709, 0.81650, 0, 1) \\
(p, T, u_r, u_{i\theta}, \lambda)_o = (1, 1, 0, 0, 1)
\end{cases}
\]

(14)

which satisfy the Hugoniot relations for detonation wave. Here the suffixes \(i\) and \(o\) index two parts, \(10000 \leq r \leq 10000.1\) and \(10000.1 < r \leq 10002\), in an annular area, respectively. The inner radius is given large enough, so that the curvature becomes negligible and the polar coordinates revert locally to Cartesian coordinates. With this condition, the simulation
Figure 2: physical quantities of steady detonation wave at time $t = 0.25$, with radial range $10000.8 \leq r \leq 10001$: (a) $\rho$, (b) $T$, (c) $P$, (d) $u_r$, (e) $\lambda$.

results can be compared to the analytic solutions of the 1-dimensional steady detonation wave. Other parameters are $\tau = 10^{-7}$, $N_r \times N_\theta = 2000 \times 3$, $\omega_1 = 1$, $\omega_2 = 50$.

Figure 2 gives LB simulation results, CJ results $[1, 4, 5]$ and ZND results $[1, 6, 7, 8]$ of physical quantities ($\rho, T, P, u_r, \lambda$) at time $t = 0.25$, with radial range $10000.8 \leq r \leq 10001$, respectively. The solid lines with squares are for LB simulation results, the dashed lines are for analytic solutions of CJ theory, and the solid lines are for analytic solutions of ZND theory. The simulation physical quantities after detonation wave are ($\rho, T, u_r, u_\theta, \lambda$) = (1.36128, 2.58909, 0.818334, 0, 1). Comparing them with CJ results gives the relative differences 0.2%, 0.3%, 0.2%, 0% and 0%, respectively. Panels (a)-(e) show that the LB simulation results have a satisfying agreement with the ZND results in the area behind von Neumann peak. There are few differences between them. Physically, the analytic solutions of ZND theory here ignore the viscosity and heat conduction, and the von Neumann peak is simply treated as a strong discontinuity. Furthermore, the relative difference is 0.5% between the simulation detonation velocity $D = 3.08$ and the analytic solution $D = 3.09557$. In sum, the current LB model works for detonation phenomenon.
3.2.2. Nonequilibrium in steady detonation wave

Figure 3 gives the physical quantities and their gradients versus radius at time $t = 0.25$, with radial range $10000.85 \leq r \leq 10000.95$. Three vertical lines are shown, from left to right, to guide the eyes for the rarefaction area, the von-Neumann peak and the pre-shocked area, respectively. Panel (a) shows that the maximum values of density, temperature, pressure, velocity do not exactly coincide. The radial positions of their maximum values are $R_\rho = 10000.9195$, $R_T = 10000.9045$, $R_P = 10000.9175$, $R_u = 10000.9195$. Panel (b) shows that the largest absolute values of $\nabla \rho$, $\nabla T$, $\nabla P$, $\nabla u$ are at the pre-shocked area, their second largest values are at the rarefaction area, and their vales are close to zero at the von-Neumann peak.

Figure 4 shows the central moments and their non-equilibrium manifestations in the case corresponding to Fig.3. The simulation results of $M_2^*(f_{ki})$, $M_3^*(f_{ki})$, $M_{3,1}^*(f_{ki})$, $M_{1,2}^*(f_{ki})$, $M_2^{eq}(f_{ki})$, $M_3^{eq}(f_{ki})$, $M_{3,1}^{eq}(f_{ki})$, $M_{1,2}^{eq}(f_{ki})$, $\Delta_2^*$, $\Delta_3^*$, $\Delta_{3,1}^*$, $\Delta_{4,2}^*$ are shown in Figs.4 (a)-(l), respectively. The vertical lines in Figs.4 (i)-(l) coincide with the ones in Fig.3. It’s easy to get from Fig.4 that, the non-equilibrium system is mainly around the von-Neumann peak. The departure of the system from its equilibrium around the leftmost line is opposite the one around the rightmost line. Physically, the former is under shock effect, whereas the latter under rarefaction effect. Furthermore, both $\Delta_{2,rr}^*$ and $\Delta_{2,\theta\theta}^*$ are close to zero at the von-Neumann peak, i.e., the internal kinetic energy in different degree of the freedom approximately equals to each other at the von-Neumann peak. Comparing Fig.3 (b) with Fig.4...
Figure 4: The simulation results of $M^*_m(f_{ki})$, $M^*_m(f^e_{ki})$ and $\Delta^*_m$ in the same case as Fig.3.

(i) gives that the internal kinetic energies in different degrees of freedom show the maximum difference at the inflexion point where the pressure has the largest spatial derivative.

Around the leftmost line in Fig.4(i), $\Delta^*_2,rr$ shows a negative peak and $\Delta^*_2,\theta\theta$ shows a positive peak with the same amplitude, which implies that the distribution function $f(v_r)$ is “thinner” and “higher” than the Maxwellian $f^e$, and $f(v_\theta)$ is “fatter” and “lower”. The simulation results of $\Delta^*_3$ in Fig.4(j) and $\Delta^*_3,1$ in Fig.4(k) indicate that $f(v_\theta)$ is symmetric, and the $f(v_r)$ is asymmetric. The portion of $f(v_r)$ for $v_r > 0$ is “fatter” than that for $v_r < 0$. Figure 5(a) shows the sketch of the actual distribution functions, $f(v_r)$, $f(v_\theta)$ and the Maxwellian $f^e$.

For the rightmost line in Fig.4 similarly, Fig.5(b) shows the sketch of the actual distribution functions, $f(v_r)$, $f(v_\theta)$ and the Maxwellian $f^e$. It can be found that $f(v_r)$ is “fatter” and “lower” than the Maxwellian $f^e$, while $f(v_\theta)$ is “thinner” and “higher”. $f(v_\theta)$ is symmetric, while $f(v_r)$ is asymmetric. The portion of $f(v_r)$ for $v_r > 0$ is “fatter” and the portion of $f(v_r)$ for $v_r < 0$ is “thinner”.

Moreover, the simulation result $\Delta^*_2,r\theta = 0$ in Fig.4(i) indicate that the contours of the
Figure 5: The sketch of the Maxwellian and actual distribution functions versus velocity $v_r$ and $v_\theta$, respectively. (a) the distribution functions at the leftmost line, (b) the distribution functions at the rightmost line. The long-dashed line is for distribution function $f(v_r)$, the shot-dashed one is for distribution function $f(v_\theta)$, and the solid line is for $f^{eq}$.

Figure 6: The sketch of contours of the actual distribution functions in velocity space $(v_r,v_\theta)$. Figure (a) and (b) show the recovered distribution function contours at the leftmost and rightmost line, respectively.

Figure 7: The sketches of the actual distribution functions in velocity space $(v_r,v_\theta)$. Figures (a) and (b) show the recovered distribution functions at the leftmost and rightmost lines, respectively.
actual distribution function in velocity space \((v_r, v_θ)\) is symmetric about the \(v_r\)-axis or/and \(v_θ\)-axis. The above analysis suggests that \(v_r\)-axis is the symmetric axis. Figure 6 shows the sketch of contours of the actual distribution function. Combining Figs. 5 and 6 gives Fig. 7, which shows the sketch of the actual distribution function in velocity space \((v_r, v_θ)\).

3.3. Simulation of implosion

For the case of implosion, the initial physical quantities are:

\[
\begin{align*}
\rho, T, u_r, u_θ, \lambda & \quad \text{(a)} \\
\rho, T, u_r, u_θ, \lambda & \quad \text{(b)} \\
\rho, T, u_r, u_θ, \lambda & \quad \text{(c)} \\
\rho, T, u_r, u_θ, \lambda & \quad \text{(d)} \\
\rho, T, u_r, u_θ, \lambda & \quad \text{(e)} \\
\rho, T, u_r, u_θ, \lambda & \quad \text{(f)} \\
\end{align*}
\]

\[
\begin{align*}
\left(\rho, T, u_r, u_θ, \lambda\right)_i &= (1, 1, 0, 0, 0) \\
\left(\rho, T, u_r, u_θ, \lambda\right)_o &= (1.5, 1.55556, -0.666667, 0, 1),
\end{align*}
\]  

where the suffixes \(i\) and \(o\) index areas \(0 \leq r \leq 0.098\) and \(0.098 < r \leq 0.1\), respectively. Other parameters are \(\tau = 10^{-5}\), \(N_r \times N_θ = 100 \times 3\), \(ω_1 = 1\), \(ω_2 = 100\).

Figure 8 shows physical quantities along radius in implosion process: (a) density; (b) temperature; (c) pressure; (d) radial velocity; (e) the parameter for chemical reaction process;
(f) $\Delta^*_{2,rr}$. There are two stages in implosion process. In the former stage, the detonation travels inwards, the material behind the detonation front moves inwards, and the density, temperature and pressure behind detonation wave increase continuously due to the disc geometric effect. When the detonation wave reaches the center, the density, temperature and pressure increase monotonically along radius. Meanwhile, the velocity reduces to zero gradually and then point outwards. In the latter stage, the detonation wave travels outwards. As the chemical reaction completes, the detonation wave becomes a shock wave. The velocity before the shock front points inwards and the one after the shock front points outwards. So the density, temperature and pressure before shock front still increase continuously, and those behind the front reduce.

In addition, Fig.8 (f) shows that the departure of the system from equilibrium increases (reduces) when the detonation or shock wave becomes stronger (weaker). Specially, the value of $\Delta^*_{2,rr}$ shows a crest and a trough from the time $t = 0.000$ to $t = 0.039$. The crest results from compression effect ahead of the detonation front, while the trough results from rarefaction effect behind. At the time $t = 0.042$, the value of $\Delta^*_{2,rr}$ is positive at the crest, negative on both sides of the crest. From $t = 0.042$ to 0.060, it is also positive at the crest and negative behind. In fact, $\Delta^*_{2,rr}$ is always positive at the shock wave and negative at the rarefaction wave, which can be seen as a criterion to distinguish the two waves. Furthermore, the system at the disc center is always in its thermodynamic equilibrium.

3.4. Simulation of explosion

For the case of explosion, the initial physical quantities are:

$$\begin{cases}
(r, T, u_r, u_\theta, \lambda)_i = (1.5, 1.55556, 0.666667, 0, 1) \\
(r, T, u_r, u_\theta, \lambda)_o = (1, 1, 0, 0, 0)
\end{cases}$$

(16)

where the suffixes $i$ and $o$ index areas $0 \leq r \leq R_1$ and $R_1 < r \leq R$, respectively. Here $\tau = 10^{-5}$, $\omega_1 = 1$, $\omega_2 = 50$. Figures 9-11 show the evolution of physical quantities ($\rho$, $T$, $P$, $u_r$, $\lambda$, $\Delta^*_{2,rr}$) versus radius. Figure 9 corresponds to parameters $R_1 = 0.010$, $R = 0.5$, $N_r \times N_\theta = 500 \times 3$; Fig.10 corresponds to parameters $R_1 = 0.034$, $R = 1.0$, $N_r \times N_\theta = 1000 \times 3$; Fig.11 corresponds to parameters $R_1 = 0.050$, $R = 2.0$, $N_r \times N_\theta = 2000 \times 3$. 
Figure 9: For the case $R_3 = 0.010$, physical quantities versus radius in explosion process at times, $t = 0.00$, 0.01, 0.15 and 0.30, respectively: (a) $\rho$; (b) $T$; (c) $P$; (d) $u_r$; (e) $\lambda$; (f) $\Delta^2_{rr}$. 
Figure 9 shows the extinction phenomenon. The area of initial reacted reaction is very small, i.e., the initial energy is not enough to trigger the detonation. The energy propagates outward in the form of disturbance wave with amplitude decreasing gradually. The wave dissipates and vanishes finally. It’s easy to get from Fig 9 (e) that \( \lambda \) only has a little change at the beginning. The reason is that the initial temperature of reacted reaction is higher than the temperature threshold \( T_{th} \) and there is a little chemical reaction at the start. The rate of chemical energy released is smaller than the rate of heat dissipated under the disc geometric effect. Consequently, the energy of disturbance wave reduces gradually, which leads to extinction. Figure (f) shows that the system has only a small departure from equilibrium at the start. The departure reduces gradually and vanishes finally.

Figure 10 shows that (i) A disturbance wave travels outwards from \( t = 0.000 \) to \( t = 0.205 \). Part reactant reacts around the disturbance wave. The released chemical energy is added into the disturbance wave, meanwhile the thermal energy within disturbance wave disperses...
to its adjacent area. The disturbance wave becomes wider in both radical and azimuthal directions under disc geometric effect, and the maximum values of density, temperature, pressure and velocity reduce. The value of $\Delta^*_{2,rr}$ shows a crest at the disturbance wave and a trough behind. (ii) The perturbation wave is transformed into detonation wave from $t = 0.205$ to $0.335$. The heat release rate of chemical reactant increases sharply. The physical quantities ($\rho$, $T$, $P$, $u_r$) increase suddenly. Meanwhile the number of crest (trough) of $\Delta^*_{2,rr}$ increases from one to two. (iii) The implosion and explosion waves coexist from $t = 0.335$ to $0.385$. With amplitude defined as the distance from the crest to trough of $\Delta^*_{2,rr}$, it is found that the amplitudes at the implosion and explosion waves increase dramatically, especially the former one from $7.98 \times 10^{-4}$ to $1.90 \times 10^{-2}$. For the purpose of a clear view, the plot of $\Delta^*_{2,rr}$ at the time $t = 0.385$ is given specially within panel (f). (iv) From $t = 0.385$ to $0.550$, the implosion wave has passed the center of the disc, then travels outwards and changes into a shock wave with the completion of chemical reaction. It is then transformed into a perturbation wave, dissipates and vanishes finally. While the explosion wave propagates outwards and its peak rises further. The amplitude of $\Delta^*_{2,rr}$ at the implosion wave reduces, and the one at the explosion wave increases.

Figure 11 shows a direct explosion phenomenon with ignition energy large enough. Panel (a) shows that the density is lower inside the detonation front than the one outside due to the disc geometric effect. Panels (b)-(c) shows higher temperature and pressure inside. Panel (d) shows that the velocity inside is close to zero. Panel (e) shows that chemical reaction steadily proceeds. Panel (f) shows that the amplitude of $\Delta^*_{2,rr}$ increases gradually. The detonation wave becomes wider and wider in both radical and azimuthal directions.

In fact, there is competition between the chemical reaction, macroscopic transportation, thermal diffusion and the geometric convergence or divergence in the detonation phenomenon. The chemical reaction increases the temperature while the thermal diffusion decreases the temperature around the detonation wave. If there is enough thermal energy transformed from chemical energy, the detonation proceeds; otherwise, extinguishes. Special in explosion case, if the geometric divergence effects dominate, extinction will occur; with the the combustion front propagating outwards, geometric divergence makes less effect, the existing part combustion may result in complete combustion, even detonation.
Figure 11: For the case $R_1 = 0.034$, physical quantities versus radius in explosion process at times, $t = 0.00$, 0.03, 0.45 and 0.90, respectively: (a) $\rho$; (b) $T$; (c) $P$; (d) $u_r$; (e) $\lambda$; (f) $\Delta^*_{2,rr}$. 
4. Conclusions and discussions

A polar coordinate Lattice Boltzmann Kinetic Model (LBKM) for detonation phenomena is presented. Within the model the fluid behavior is simulated by a finite-difference LBKM in polar coordinates, and the chemical reaction is described by Cochran’s rate function. A combined scheme is used to treat with the LB equation and the Cochran’s rate equation. Both the temporal evolution of the collision effects in the LB equation and the temporal evolution of chemical reaction in Cochran’s rate equation are calculated analytically. Both the convection terms in the LB equation and Cochran’s rate equation are treated using the first-order upwind scheme. From the numerical point of view, compared with the LBKM in Ref. [41], the present model has the same accuracy but is simpler. From the physical or chemical point of view, compared with the Lee-Tarver model used in previous work [34], the pressure effects on the reaction rate is taken into account in the Cochran’s rate function.

Compared with the previous work in Ref. [41], the inner boundary condition for the disc computational domain is treated more naturally. In Ref. [41] the disc computational domain is approximated by a annular domain where the inner radius approaches zero. Consequently, one needs to construct ghost nodes for the inner boundary condition. In this work the center of the disc computational domain is considered as a inner point of the system. For periodic system, no ghost node is needed for the inner boundary condition. Other boundaries are treated with the same method as [41].

The simulation results of physical quantities in the steady detonation process have a satisfying agreement with analytical solutions. Typical implosion and explosion phenomena are simulated. By changing initial ignition energy, we investigate three cases of explosion, including a case with extinction phenomenon. It is interesting to find that the geometric convergence or divergence effect makes the detonation procedure much more complex. The competition between the chemical reaction, the macroscopic transportation, the thermal diffusion and the geometric convergence or divergence determines the ignition process. If there is enough thermal energy transformed from chemical energy, the detonation proceeds; otherwise, extinguishes. Specially in explosion case, if the geometric divergence effects dominate, extinction will occur; with the combustion front propagating outwards, geometric divergence makes less effect, the existing part combustion may result in complete combustion, even
detonation.

Finally, the non-equilibrium behaviors in detonation phenomenon are investigated via the velocity moments of discrete distribution functions. The system at the disc center is always in its thermodynamic equilibrium. The internal kinetic energies in different degrees of freedom show the maximum difference at the inflexion point where the pressure has the largest spatial derivative. The influence of shock strength on the reaction rate and the influences of both the shock strength and the reaction rate on the departure amplitude of the system from its local thermodynamic equilibrium are probed. The departure from equilibrium in front of von-Neumann peak results from shock effect, while the one behind the peak results from rarefaction effect. The departure increases when the shock or rarefaction effect increases. Specially, the value of $\Delta_{2,rr}^*$ is positive at shock wave and negative at the rarefaction wave, which can be seen a criterion to distinguish the two waves. What’s more, the main behaviors of actual distribution functions around the detonation wave are recovered from the numerical results of high-order moments of the discrete distribution function.

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