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CORRECTIONS TO THE COLLISION TERM IN THE BGK BOLTZMANN EQUATION*

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With the discrete method of the hexagonal cell and three different velocities of particle population in each cell, a two-dimensional lattice Boltzmann model is developed in this paper.[1,2] The collision operator in the Boltzmann equation is expanded to fourth order using the Taylor expansion.[3,4] With this model, good results have been obtained from the numerical simulation of the reflection phenomenon of the shock wave on the surface of an obstacle, and the numerical stability is also good. Thus the applicability of the $D2Q19$ model is verified.

Keywords: lattice Boltzmann model, collision operator, shock wave
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I. INTRODUCTION

From a microscopic point of view, the lattice Boltzmann equation (LBE) models define physical variables of macroscopic fluid in spatial discrete cells with the moment of particle populations. For example, the fluid mass in a discrete cell is equivalent to the sum of the mass of each particle population, the fluid momentum is equivalent to the sum of the momentum of each particle population, and the kinetic energy and internal energy of the fluid are also equivalent to the sum of the kinetic energy of each particle population. It is obvious that the dynamic and thermodynamic physical processes described in the LBE model are not simplified, but on the contrary the model reveals more clearly on the microscopic level that the macroscopic physical behaviour of the fluid is the average of the random thermal motion of particles.

The Boltzmann equation is a complicated differential and integral equation, and it is difficulty to find its analytical solution even in very simple cases. So, at present, the linear simplified Bhatnagar–Gross–Krook (BGK) Boltzmann equation is adopted widely.[3] This study refers to the idea of Chen,[4] that the collision operator in the Boltzmann equation is expanded to fourth order with a Taylor series and thereby a two-dimensional $D2Q19$ lattice Boltzmann model is established. The reflection phenomenon of the shock wave on the surface of an obstruction is simulated using the $D2Q19$ model. The numerical result is consistent with the experiment,[5] and the numerical stability is also good.

II. LATTICE BOLTZMANN MODEL

The equation governing the motion of particle population is the Boltzmann equation

$$f_{ki}(r_\alpha + c_{ki\alpha}\delta t, t+\delta t) - f_{ki}(r_\alpha, t) = \Omega(f_{ki}), \quad (1)$$

where f_{ki} is a velocity distribution function of particles, i is the directional number of moving particles, k represents types of fluid, and $c_{ki\alpha}$ is the velocity of particles. $c_{ki\alpha}$ has the same modulus in all directions, $|c_{ki\alpha}| = c_k$=const. α represents the index of coordinates, δt is discrete time size, and Ω is a collision operator. Based on the Chapman–Enskog expansion method, the velocity distribution function is asymptotically expanded in the domain of local equilibrium distribution $f_{ki}^{(0)}$, and the following can be derived

$$\begin{aligned} f_{ki} &= f_{ki}^{(0)} + f_{ki}^{neq}; \\ f_{ki}^{neq} &= f_{ki}^{(1)} + f_{ki}^{(2)} + \cdots + f_{ki}^{(n)}; \\ f_{ki}^{(n)} &= O(\varepsilon^{(n)}); \\ \partial^{(n)} f_{ki}^{(n)} &= O(\varepsilon^{(n+1)}), \end{aligned} \quad (2)$$

where f_{ki}^{neq} is a non-equilibrium component. The local

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equilibrium distribution is given by[6,7]

$$\begin{aligned} f_{ki}^{(0)} =& W_i\rho(1 - 2Ec_{ki\alpha}u_\alpha + 2E^2k_{ki\alpha}c_{ki\beta}u_\alpha u_\beta \\ &+ Eu^2 - 2E^2c_{ki\alpha}u_\alpha u^2 \\ &- \frac{4}{3}E^3c_{ki\alpha}c_{ki\beta}c_{ki\chi}u_\alpha u_\beta u_\chi). \end{aligned} \tag{3}$$

Making a Taylor expansion of Ω_{ki} at $f_{ki} = f_{ki}^{(0)}$ [4] and taking the accuracy to the fourth order, we obtain

$$\begin{aligned} \Omega(f_{ki} =& \Omega(f_{ki}^{(0)}) + \frac{\partial\Omega}{\partial f_k}f_{ki}^{neq} + \frac{1}{2!}\frac{\partial^2\Omega}{\partial f_k^2}(f_{ki}^{neq})^2 \\ &+ \frac{1}{3!}\frac{\partial^3\Omega}{\partial f_k^3}(f_{ki}^{neq})^3 + O((f_{ki}^{neq})^4). \end{aligned} \tag{4}$$

In terms of the Chapman–Enskog theory,[4] $\Omega(f_{ki}^{(0)}) = 0$. Like the coefficient of Burnett, it is difficulty to give an analytical solution for the collision operator Ω. With reference to Chen,[4] we take

$$\left.\frac{\partial^n\Omega}{\partial f_{ki}^n}\right|_{f_{ki}=f_{ki}^{(0)}} = \left(-\frac{1}{\tau}\right)^n, \tag{5}$$

where τ is the coefficient of non-dimensional relaxation time. The establishment of the relationship between particle populations and macroscopic fluid parameters require the satisfaction of the conservation laws of mass and momentum, the law of energy relation,[1,2] as well as the energy flux relation

$$\left(\frac{1}{2}\rho u^2 + \rho e + P\right)u_\alpha = \frac{1}{2}\sum_k\sum_i f_{ki}^{(0)}c_k^2c_{ki\alpha}. \tag{6}$$

Taking the hexagonal cell as shown in Fig.1(a), there are three kinds of particles with different velocities in each discrete cell. The weight W_i and coefficient E are found from the above conservation formulae

$$\begin{aligned} W_0 =& 1 - \frac{4e^3(D+4)(D+2) + 49eD^2c_1^4 - 28e^2Dc_1^2(D+2)}{18D^2c_1}, \\ W_1 =& \frac{2e^3(D+4)(D+2) + 18eD^2c_1^4 - 13e^2Dc_1^2(D+2)}{6bD^2c_1^6}, \\ W_2 =& \frac{20e^2Dc_1^2(D+2) - 4e^3(D+4)(D+2) - 9eD^2c_1^4}{30bD^2c_1^6}, \\ W_3 =& \frac{2e^3(D+4)(D+2) + 2eD^2c_1^4 - 5e^2Dc_1^2(D+2)}{90bD^2c_1^6}, \\ E =& -\frac{D}{4e}; \quad P = \frac{2}{D}\rho e; \quad (D = 2, c_3 = 3c_1, c_2 = 2c_1). \end{aligned}$$

Here P is the pressure, ρ is the density of fluid, e is the internal energy of fluid per unit mass, D is the space dimension, and b is the directional number of lattice.

Ⅲ. NUMERICAL EXPERIMENT AND CONCLUSION

The numerical simulation tests the numerical stability and applicability of $D2Q19$ by simulating the reflection of the shock wave on the surface of an obstruction.

Figure 1(b) shows the structural characteristic scales of fluid field. The 200 by 500 area on the left is the high-pressure zone. Initial conditions are set to (ρ_L, u_α, e_L)=$(3.0\rho_R, 0.0, 0.65)$. Other areas are low-pressure zones and initial conditions are taken as (ρ_R, u_α, e_R)=(1.0, 0.0, 0.65). The coefficient of non-dimensional relaxation time τ=0.60. The no-slip condition is applied on the boundaries, and the open side in figure 1(b) is set as

$$\frac{\mathrm{d}\rho}{\mathrm{d}x} = 0; \frac{\mathrm{d}Vx}{\mathrm{d}x} = 0; \frac{\mathrm{d}Vy}{\mathrm{d}x} = 0.$$

Numerical results of the reflection effect of the shock wave are given in Fig.3. The figures clearly show the propagation of the shock wave and its reflection on the turning corner. These numerical results are consistent with experimental results.[5] Figure 2(a) presents the pressure distribution along the X-direction in the fluid field, showing the feature of propagation and contact discontinuity of the Mach wave. Figure 2(b) shows the distribution of the Mach number along the X-direction at the position of the dashed line Mv in the fluid field. It can be seen that there is an obvious velocity jump on the inclined plane, which is similar to the contraction section of the Laval jet pipe. The jump in a variable cross-section tube can be explained, using a one-dimensional differential equation which is both isoentropic and stable

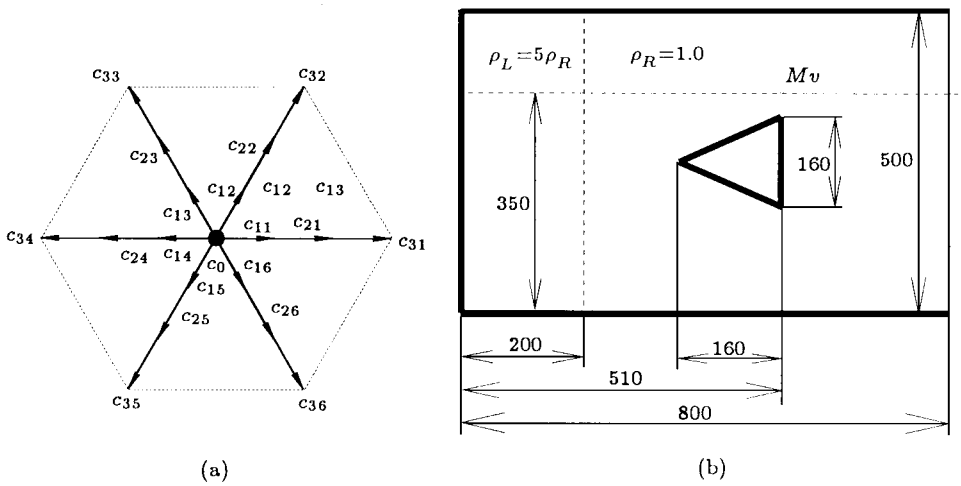


Fig.1. (a) A two-dimensional discrete hexagonal cell of LBE $D2Q19$; velocity of particles $c_{2i} = 2c_{1i}$, $c_{3i} = 3c_{1i}$. (b) Sketch of the fluid field.

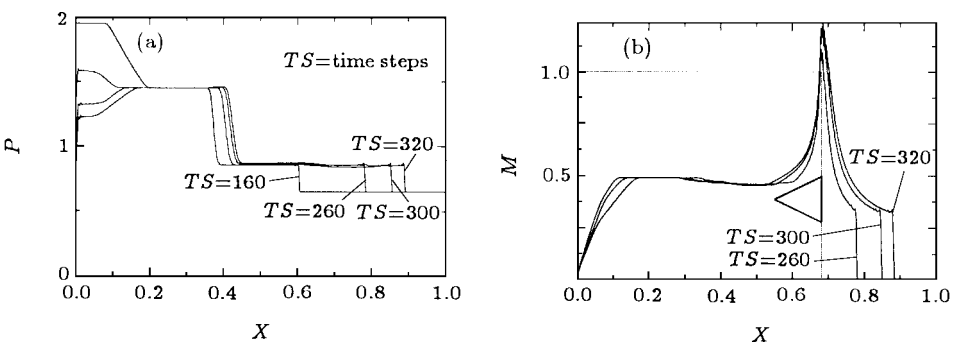


Fig.2. (a)Pressure distribution along dashed line Mv (figure 1(b)). (b) Distribution of Mach number $M = Vx/a$ at corresponding position (Vx is the flow velocity along the X coordinate axis, a is sound speed $a^2 = 2e/D$), TS are integral time steps.

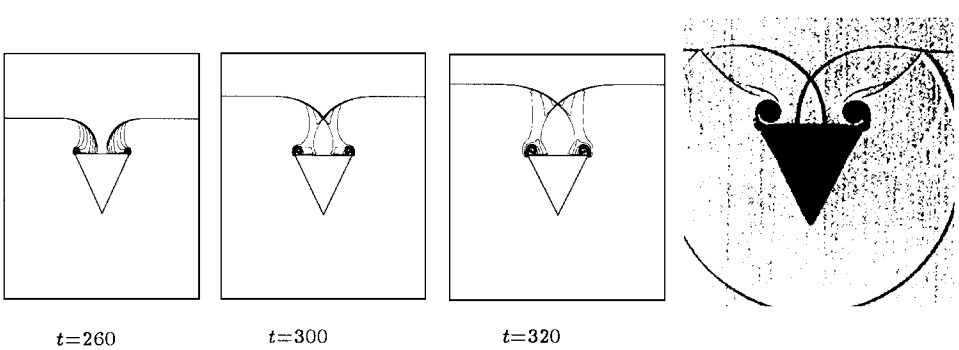


Fig.3. Comparison of the numerical results of the $D2Q19$ model with the experimental results;[5] t is integral time steps, the contour is density distribution.

$$(M^2 - 1)\frac{\mathrm{d}V}{V} = \frac{\mathrm{d}A}{A}, \tag{7}$$

where A is cross-sectional area. The expression shows that, if the flow speed is subsonic, $M < 1$ then $M^2 - 1 < 0$, $\mathrm{d}V/V$ and $\mathrm{d}A/A$ are necessarily of different signs, with opposite variability. The gradual decrease of the cross section results in the gradual increase of gas velocity so, on the turning corner $\mathrm{d}A/A$=0, the gas velocity increases to critical status M=1. At the time of gas flowing the turning corner, it undergoes an instantaneous expansion and accel-

eration process and reaches supersonic status. After the acceleration, it enters the frictional tube section, $\mathrm{d}A/A{=}0$. In the frictional tube section, there is always $(M^2-1)\mathrm{d}V/V<0$, i.e., $\mathrm{d}V/V$ always has different signs from M^2-1, so the supersonic gas velocity will be attenuated gradually.

In summary, the numerical simulation of the reflection effect of the shock wave on the surface of an obstruction gives a good result by using the $D2Q19$ model. The numerical stability is also good. Thus the applicability of the lattice Boltzmann model is verified both in theory and by experiment.

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