

Nonequilibrium Bhatnagar–Gross–Krook model for nitrogen shock structure

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This Brief Communication is about the study of diatomic gas shock structure based on the nonequilibrium gas-kinetic Bhatnagar–Gross–Krook (BGK) model, where an additional rotational energy relaxation equation is added. The BGK Navier–Stokes flow solver is extended to solve the nonequilibrium gas kinetic model. The numerical solutions are compared with the experiment measurements and direct simulation Monte Carlo solutions. © 2004 American Institute of Physics. [DOI: 10.1063/1.1783372]

The objective of this study is to develop a gas-kinetic scheme for the rarefied high energy flow application. It is well recognized that the Navier–Stokes equations of the classical hydrodynamics are incapable of accurately describing shock wave phenomena. In order to improve the Navier–Stokes solutions, much effort has been paid on the construction of higher-order hydrodynamic equations based on the Chapman–Enskog expansion, such as the Burnett equations.^{1,2} For diatomic gas, such as nitrogen, besides the rarefied gas effect the nonequilibrium phenomenon related to the translational and rotational degrees of freedom has to be accounted as well. For example, Lumpkin and Chapman extended their modified Burnett equations in the nitrogen shock structure calculation.³ In this Brief Communication, we are going to study the nitrogen shock structure based on the nonequilibrium gas-kinetic Bhatnagar–Gross–Krook (BGK) model. The nonequilibrium rotational energy model is based on the Jeans' equation.⁴ The simulation results are compared with the experimental and direct simulation Monte Carlo (DSMC) solutions.

The model equation we are going to solve is the generalized BGK model,⁵

$$f_t + uf_x = \frac{g - f}{\tau}, \quad (1)$$

where f is the gas distribution function and g is the equilibrium state approached by f . Both f and g are functions of space x , time t , particle velocity u , and translational ξ and rotational η degrees of freedom. For a diatomic gas, the equilibrium state is an ellipsoid Maxwellian distribution,

$$g = \rho \left(\frac{\lambda_t}{\pi} \right)^{3/2} \left(\frac{\lambda_r}{\pi} \right) e^{-\lambda_t[(u-U)^2 + \xi^2] - \lambda_r \eta^2},$$

where ρ is the density, U is the macroscopic flow velocity in the x direction, λ_t is related to the translational temperature

$m/2kT_t$, and λ_r to the rotational temperature $m/2kT_r$. The nitrogen gas has $\xi^2 = \xi_1^2 + \xi_2^2$ and $\eta^2 = \eta_1^2 + \eta_2^2$ to account for two translational degrees of freedom in the y and z directions and two rotational ones. Note that the particle collision time τ determines the viscosity and heat conduction coefficients. The relation between mass ρ , momentum ρU , total energy ρE , and internal energy ρE_r densities with the distribution function f is

$$W = \begin{pmatrix} \rho \\ \rho U \\ \rho E \\ \rho E_r \end{pmatrix} = \int \psi f du d\xi d\eta,$$

where ψ has the components

$$\psi = \left[1, u, \frac{1}{2}(u^2 + \xi^2 + \eta^2), \frac{1}{2}\eta^2 \right]^T.$$

Since only mass, momentum, and total energy are conserved during particle collisions, f and g satisfy the condition

$$\int (g - f) \psi_\alpha du d\xi d\eta = S = (0, 0, 0, s)^T, \quad \alpha = 1, 2, 3, 4. \quad (2)$$

The source term s in the internal energy equation is $s = \rho(E_r^{\text{eq}} - E_r)/Z_R\tau$. Here $Z_R\tau$ is the relaxation time for rotational energy to get equilibrium. Since it takes longer time for the rotational energy than the translational one to settle to the equilibrium, the rotational collision number Z_R usually has a value between 1 and 10. The equilibrium energy ρE_r^{eq} is determined by

$$\rho E_r^{\text{eq}} = \rho/\lambda^{\text{eq}}$$

and

$$\lambda^{\text{eq}} = \frac{5}{4} \frac{\rho}{\rho E - \frac{1}{2}\rho U^2}.$$

The numerical method developed for Eq. (1) is a finite volume method,

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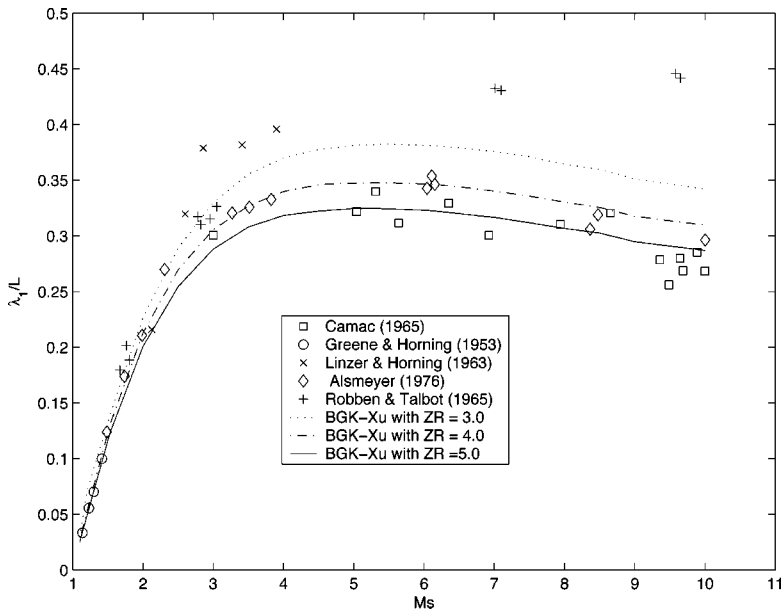


FIG. 1. Reciprocal shock thickness vs Mach number for nitrogen gas. All symbols are experimental results. The theoretical results are based on the nonequilibrium BGK-Xu scheme for the nonequilibrium BGK model. The lines (dotted, dot-dash, and solid) correspond to $Z_R=3, 4, 5$, respectively.

$$W_j^{n+1} = W_j^n + \frac{1}{\Delta x} \int_0^{\Delta t} [F_{j-1/2}(t) - F_{j+1/2}(t)] dt + S_j^n \Delta t, \quad (3)$$

where W_j^n is the cell averaged mass, momentum, total energy, and internal energy, and $F_{j+1/2}$ is the corresponding fluxes at a cell interface by solving Eq. (1). Note that Δt is the time step $\Delta t = t^{n+1} - t^n$, and S_j^n is the source term for the internal energy. The above scheme is mainly about the evaluation of the fluxes based on the integral solution of the BGK model (1), where the so-called BGK Navier–Stokes (BGK-NS) scheme⁶ can be extended here to include the internal energy equation easily. The main difference between the current nonequilibrium BGK-NS method and the equilibrium BGK-NS method in Ref. 6 is that two temperatures λ_t and λ_r are used in the equilibrium state and an additional source term is included in Eq. (3) to update the rotational energy. On the contrary, the equilibrium BGK-NS code has only a single temperature and a constant $\gamma=1.4$ is used. In order to simulate the flow with any realistic Prandtl number, a modification of the heat flux in the energy transport, such as that used in Ref. 6, is also implemented in the current calculation.

In order to include the translational rarefied gas effect in the gas-kinetic model, a generalized particle collision time τ^* is constructed in Ref. 7. The basic idea there is to assume a solution of the BGK model, i.e., $f = g - \tau^*(g_t + u g_x)$, and put it back into the BGK equation, from which a generalized particle collision time τ^* can be derived,

$$\tau^* = \tau / (1 + \tau \langle D^2 g \rangle / \langle D g \rangle), \quad (4)$$

where $\langle (\dots) \rangle = \int (u - U)^2 (\dots) du d\xi d\eta$, $Dg = g_t + u g_x$, and $D^2 g = g_{tt} + 2u g_{xt} + u^2 g_{xx}$. Here τ depends on the macroscopic variables through $\tau p = \mu_\infty (T/T_\infty)^\omega$, and the generalized τ^* will depend not only on the macroscopic variables, but also their gradients. Or, we can consider τ^* as a generalized constitutive relation for the translational nonequilibrium flow. The nonequilibrium BGK-NS scheme with the implementation of τ^* is named the nonequilibrium BGK-Xu method.

For nitrogen gas, the viscosity coefficient is given by $\mu = \mu_\infty (T/T_\infty)^\omega$, where $\omega=0.722$ and it corresponds to $\nu=10$ for the power index of the intermolecular force law.⁸ The Prandtl number for nitrogen gas is $Pr=0.72$. In our calculation, the local particle collision time τ is first evaluated according to $\tau = \mu/p$. Then, the value τ^* is obtained from Eq. (4).

In summary, in order to capture the nonequilibrium property and the rarefied gas effect of nitrogen shock structure, we have tried the following schemes. The first scheme is the equilibrium BGK-NS (Ref. 6) for nitrogen gas, which is basically to solve the equilibrium Navier–Stokes equations with $T_r = T_t$ and $Z_R = 1.0$ in the BGK model. The second scheme solves the rotational nonequilibrium BGK model with different translational and rotational temperatures and a constant rotational collision number Z_R . The collision time for this scheme is still based on the continuum assumption, such as $\tau = \mu/p$. This scheme is called nonequilibrium BGK-NS. The third scheme is the nonequilibrium BGK-NS method plus a generalized particle collision time τ^* . This scheme is called nonequilibrium BGK-Xu. All shock structures are obtained using a time accurate flow solver until a steady state is reached. In each calculation, the mesh size is chosen to make sure that there are about 20–30 points in the shock layer and the whole computational domain is covered by 200 grid points.

Studies of the shock structure are generally validated by comparing the reciprocal density shock thickness with experimental measurements. The thickness is defined as

$$L = (\rho_2 - \rho_1) / (d\rho/dx)_{\max}.$$

The above shock thickness is normalized by the upstream mean free path

$$\lambda_1 = \frac{16}{5\sqrt{\pi}} \frac{\mu_1}{\rho_1 \sqrt{2RT_1}}.$$

Figure 1 displays the results of the reciprocal thickness

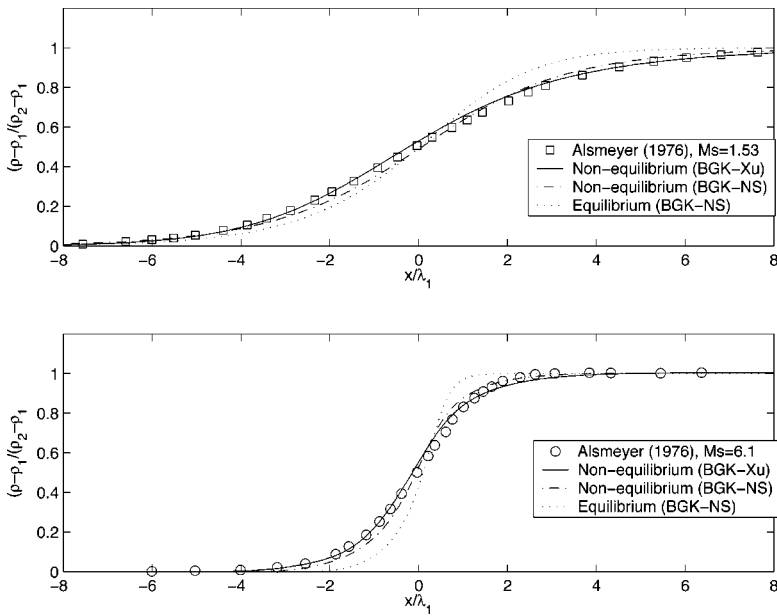


FIG. 2. Experimental and theoretical results for nitrogen shock structure with Mach numbers 1.53 (upper) and 6.1 (lower). The squares and circles are the experimental data from Alsmeyer (1976) (Ref. 9). The lines correspond different kinetic models, such as equilibrium BGK-NS (dotted), nonequilibrium BGK-NS (dot-dash), and nonequilibrium BGK-Xu (solid). $Z_R=4$ is used in all calculations.

vs Mach number based on the calculation of nonequilibrium BGK-Xu scheme. The three curves in this figure are obtained using different rotational collision number Z_R , such as 3, 4, and 5, respectively. In this figure, the experimental data was coming from the results by Alsmeyer,⁹ Camac,¹⁰ Greene and Horning,¹¹ and Linzer and Horning.¹² Similar to the argon shock structure case,⁷ the equilibrium Navier–Stokes solutions based on the equilibrium BGK-NS scheme gives a much thinner shock thickness, which are not shown here. From this figure, we can realize the effect of Z_R on the shock thickness for diatomic gas. In order to get a good match with the experimental data, the physical value Z_R should be varied from large value in the high Mach number case to the small one in the low Mach number case. In other words, the low Mach diatomic gas has a relative short relaxation time for the rotational energy to get to the equilibrium with the translational one. In order to obtain the equilibrium and nonequi-

librium effect on the shock structure, Fig. 2 presents the density distribution $\rho_n = (\rho - \rho_1) / (\rho_2 - \rho_1)$ vs x/λ_1 from three different schemes for the cases with Mach numbers $M = 1.53$ and $M = 6.1$. In all cases, $Z_R = 4.0$ is used. The symbols in Fig. 2 are the experimental data in Ref. 9. From this figure, we can observe that the rotational nonequilibrium has a significant contribution to the thickness of shock structure. But, the rarefied gas effect with the modification of τ^* has marginal impact. Basically, there is not much difference between the results from the nonequilibrium BGK-NS and the nonequilibrium BGK-Xu schemes at the low and modest Mach number.

Finally, in order to see the temperature T_t and T_r profiles inside a shock layer, we have used the nonequilibrium BGK-Xu scheme for the shock structure computation at Mach number $M = 11.0$ and a constant $Z_R = 5.0$. The temperature and density distributions are shown in Fig. 3, where the

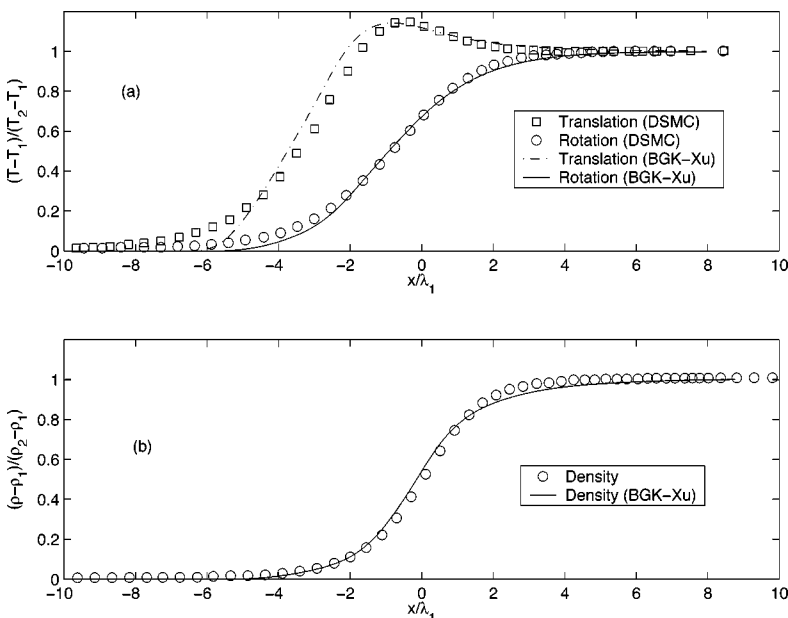


FIG. 3. Translational, rotational temperature, and density distributions for nitrogen shock layer with Mach number 11 and $Z_R = 5.0$. All lines are the results of the nonequilibrium BGK-Xu method and the symbols are the DSMC solution in Lumpkin and Chapman (1992) (Ref. 3).

symbols are coming from the DSMC simulation under the same flow condition Ref. 3. The different temperature profiles inside the shock layer are captured by the nonequilibrium BGK model. In the above simulations, we have used a constant Z_R , which is the same condition used in the DSMC calculation to match the experiments. However, the continuum techniques developed by Lumpkin¹³ must use a substantially rising value with temperature ($Z_R \approx 5$ at room temperature, $Z_R \approx 18$ at very high temperature). This is probably due to the different mechanism in the kinetic formulation here and the extended hydrodynamic equations in Ref. 13.

In this Brief Communication, we have used the nonequilibrium BGK model in the computation of diatomic gas shock structure. The gas-kinetic BGK-NS scheme is extended to solve the generalized kinetic model with rotational energy relaxation. The translational rarefied gas effect with the modification of particle collision time (constitutive relation) is also included. The reasonable agreement between the experimental data and computational results shows that the nonequilibrium BGK model with a generalized particle collision time can be used to describe nitrogen shock structure in the modest Mach numbers. The further study of the relation between the bulk viscosity approach and the relaxation model will be conducted in the near future.

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