A generalized Bhatnagar–Gross–Krook model for nonequilibrium flows

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The Bhatnagar–Gross–Krook (BGK) model approximates the collision term of the Boltzmann equation by a single relaxation process from a nonequilibrium state to an equilibrium state. From the BGK model, the Navier–Stokes, Burnett, and Super-Burnett equations can be derived. However, the success of these derived macroscopic equations in the description of highly nonequilibrium flow is limited. In order to extend the validity of the BGK model to cope with complicated physical relaxation processes, we propose a generalized BGK (GBGK) model, where the gas distribution function settles to an equilibrium state through multiple particle collisional processes. The GBGK model can be used to capture the transitional, rotational, and vibrational nonequilibrium flow phenomena. More importantly, it may provide a theoretical framework to derive new macroscopic governing equations which are valid in the near continuum flow regime. © 2008 American Institute of Physics. [DOI: 10.1063/1.2837174]

I. INTRODUCTION

It is well recognized that the derived Navier–Stokes (NS), Burnett, and Super-Burnett equations from the BGK model are incapable of accurately describing nonequilibrium flow phenomena, such as the shock wave. In order to capture the nonequilibrium physics in the transitional flow regime, we have developed gas kinetic numerical methods. First, a closed solution of the gas distribution function up to the NS order has been used to derive a generalized particle collision time, subsequent to obtaining the extended viscosity and heat conduction coefficients.¹ Later, in order to describe the nonequilibrium flow related to the molecular rotational and vibrational degree of freedom, a multiple time relaxation kinetic scheme has been introduced for the shock structure calculations.² Recently, the gas-kinetic scheme has been further extended to study the nonequilibrium multiple translational temperature.³ The numerical schemes developed in the above study give reasonable results in the transitional flow regime, such as the capturing of shock structure at different Mach numbers. Based on the above numerical experiments, we realized that the underlying physical model in the above schemes is different from the original BGK equation. In this paper, a generalized BGK (GBGK) model for the description of nonequilibrium flow will be presented.

II. GENERALIZED BGK MODEL AND ITS NUMERICAL SCHEME

The gas-kinetic Bhatnagar–Gross–Krook (BGK) model has the form,⁴

$$\frac{\partial f}{\partial t} + \mathbf{u} \cdot \frac{\partial f}{\partial \mathbf{x}} = \frac{f^{\text{eq}} - f}{\tau}, \quad (1)$$

where the distribution function f is a function of time t , spatial location $\mathbf{x}$, and particle velocity $\mathbf{u}$, and other internal degrees of freedom. The left-hand side of the above equation represents the free streaming of molecules in space, and the

right-hand side denotes the simplified collision term of the Boltzmann equation. In the BGK model, the collision operator involves a single relaxation time τ for a nonequilibrium state to evolve to an equilibrium one f^{eq} . Traditionally, based on the above BGK model, the Navier–Stokes and higher-order equations, such as Burnett and Super-Burnett, can be derived.^{5,6} Unfortunately, the higher-order equations have intrinsic physical and numerical problems in the transitional flow regime. In order to extend the capacity of the BGK model to the nonequilibrium flow regime, we can rewrite the collision term of the BGK model into two physical subprocesses,

$$\frac{\partial f}{\partial t} + \mathbf{u} \cdot \frac{\partial f}{\partial \mathbf{x}} = \frac{g - f}{\tau} + \frac{f^{\text{eq}} - g}{\tau}, \quad (2)$$

where g is a multiple temperature state between f and f^{eq} , see Fig. 1. In the above equation, the term related to $(f^{\text{eq}} - g)/\tau$ has no direct connection with f , therefore, we can consider it as a source term in the above generalized BGK (GBGK) model,

$$\frac{\partial f}{\partial t} + \mathbf{u} \cdot \frac{\partial f}{\partial \mathbf{x}} = \frac{g - f}{\tau} + Q. \quad (3)$$

The above equation shows two physical processes from a nonequilibrium state f to settle down to an equilibrium one f^{eq} . First, the nonequilibrium distribution function f relaxes to a multiple temperature state g , then g relaxes to an equal temperature Maxwellian. These two processes may have different relaxation time scales, and the specific formulation of g depends on the flow problems. For example, if we only consider the translational and rotational temperature differences, g can be defined by

FIG. 1. (Color online) Schematic description of the original and generalized BGK models.

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

where $\lambda_t = m/2kT_t$ and $\lambda_r = m/2kT_r$ are related to translational and rotational temperature. If the translational nonequilibrium state is further refined, the state g can be extended to

$$g = \frac{\rho}{(2\pi)^{3/2}} \frac{1}{|\epsilon|^{1/2}} \left(\frac{\lambda_r}{\pi} \right) \times \exp \left[-\frac{1}{2}(u_i - U_i)\lambda_{ij}(u_j - U_j) - \lambda_r \xi^2 \right],$$

where $\epsilon = \lambda^{-1}$.

In order to get a local solution of f around g , instead of using the Chapman–Enskog expansion, we can assume a closed solution

$$f = g - \tau^* Dg, \quad (4)$$

where $D = \partial_t + \mathbf{u} \cdot \partial_{\mathbf{x}}$. Substituting the above solution into the GBGK model, around g we can get

$$\tau^* = \tau / (1 + \tau D^2 g / Dg),$$

which defines a generalized particle collision time. Since $\tau D^2 g / Dg \simeq \text{Kn}$, in the continuum flow regime the modification of the particle collision time vanishes automatically. In order to remove the particle velocity dependence in τ^* , we can calculate

$$\tau^* = \frac{\tau}{1 + \tau \langle D^2 g \rangle / \langle Dg \rangle}, \quad (5)$$

where $\langle \cdots \rangle$ are moments of particle velocity, such as $(\mathbf{u} - \mathbf{U})^2$.¹ Therefore, a generalized viscosity coefficient $\tau^* p$ has been defined. If we make a Taylor expansion on the above τ^* in Eq. (4), it shows that higher order Chapman–Enskog terms have been absorbed into τ^* .

In the second relaxation stage, the multiple temperature g will relax to an equilibrium state f^{eq} . The relaxation process depends on the specific physical quantities to be considered. For example, the rotational energy of a molecule will get to equilibrium with a time scale $Z_r \tau$,^{7,8} where Z_r is the rotational collision number. For the vibrational energy, it takes a much longer time in the energy relaxation, i.e., $Z_v \tau$.⁸

In order to apply the GBGK model to study nonequilibrium flow phenomena, we can construct a finite volume scheme to update macroscopic flow variables inside each numerical cell.⁹ Taking moments of particle velocity ψ , which will be specified later, to the GBGK equation (3), we get

$$W_j^{n+1} = W_j^n + \frac{1}{\Delta x} \int_{t^n}^{t^{n+1}} (F_{j-1/2}(t) - F_{j+1/2}(t)) dt + \int_{t^n}^{t^{n+1}} \int_{x_{j-1/2}}^{x_{j+1/2}} S dt dx,$$

where the numerical fluxes at a cell interface can be obtained from the integration of the gas distribution function,

$$f = g - \tau^* Dg + \frac{\partial g}{\partial t} t, \quad (6)$$

and the source term S depends on the flow variables to be considered. The Prandtl number in the above scheme can be also modified to any value by justifying the heat flux inside $F_{j+1/2}$ across the cell interface.

III. NUMERICAL EXPERIMENTS

One of the simplest and most fundamental gas dynamic phenomena that can be used for the model validation is the structure of a normal shock wave. To illustrate the performance of the GBGK model, we first present the nitrogen shock structure, where the multiple temperature state g can be constructed as

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

where a single translational and a single rotational temperature are used. Taking the following moments on the collision term of the GBGK model:

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

which account for the mass, momentum, total energy, and the rotational energy, the source term S for the update of the macroscopic flow variables becomes

$$S = \int \psi Q du d\xi = [0, 0, 0, (E_r^{\text{eq}} - E_r) / (Z_r \tau)]^T,$$

where the equilibrium rotational energy E_r^{eq} is obtained by equalizing the translational and rotational temperature. The nitrogen shock structure studied has a Mach number 11. It was shown in Ref. 10 that Bird's DSMC results can accurately predict the translational and rotational temperature.⁸ With the same relaxation parameters as that used in the DSMC computation¹⁰ and Sutherland's law for the viscosity coefficient $\mu = \tau p$ in the determination of τ , the computational density, translational, and rotational temperature from the GBGK model is presented in Fig. 2, where a reasonable agreement with the DSMC solution has been obtained.

The next example is related to a 2D microchannel flow of a monatomic gas at low Mach numbers. In this case, the multiple temperature state g inside a rectangular channel can be approximated as

FIG. 2. (Color online) Translational, rotational temperature, and density distributions for nitrogen $M=11$ shock structure. DSMC solution (Ref. 10) vs GBGK solution.

$$g = \rho \left(\frac{\lambda_x}{\pi} \right)^{1/2} \left(\frac{\lambda_y}{\pi} \right)^{1/2} \left(\frac{\lambda_z}{\pi} \right)^{1/2} \times \exp[-\lambda_x(u-U)^2 - \lambda_y(v-V)^2 - \lambda_z(w-W)^2],$$

where λ_x , λ_y , and λ_z are related to the temperature in individual directions. Taking the moments

$$\psi = (1, u, v, \frac{1}{2}u^2, \frac{1}{2}v^2, \frac{1}{2}w^2)^T$$

for the mass, momentum, and “directional” energy, on the collision term of the GBGK model, the source term becomes

$$S = \int \psi Q du dv dw = [0, 0, 0, (E^{\text{eq}} - E_x)/\tau, (E^{\text{eq}} - E_y)/\tau, (E^{\text{eq}} - E_z)/\tau]^T,$$

which account for the mass, momentum, and energy relaxations. In the slip flow regime at Knudsen number 0.1, it is generally recognized that the Navier–Stokes equations with the slip boundary condition are capable of accurately simulating the microchannel flow. However, for the simple force and pressure driven Poiseuille flow at $\text{Kn}=0.1$, the Navier–Stokes equations give qualitatively incorrect predictions.¹¹ For example, they fail to reproduce the central minimum in the temperature and nonconstant pressure profile in the force driven case, and give opposite curvature of pressure distribution in the pressure driven case, which are predicted in the Boltzmann solution and observed in the DSMC simulations.^{12–16} With the same setup as presented in Ref. 11, the simulation results from the GBGK model are shown in Figs. 3 and 4 for the force and pressure driven cases. The temperature minimum for the averaged temperature can be clearly observed in Fig. 3 for the force driven case. This is surprising because the analysis in Ref. 14 confirms that the temperature minimum does not even appear in the Burnett order. Figure 4 shows the pressure distribution for the pressure driven case. The pressure from the GBGK model has

FIG. 3. Temperature distributions in the cross stream direction for the force driven Poiseuille flow at $\text{Kn}=0.1$.

the same curvature as that of the DSMC solution, where the standard NS solution has opposite pressure curvature.

IV. CONCLUSION

We conclude this paper with the following remarks about the GBGK model:

(1) The GBGK model uses two relaxation processes to approximate the Boltzmann collision term. In the continuum flow regime, the GBGK will recover the standard BGK model as g being close to f^{eq} .

(2) Based on the Chapman–Enskog expansion, the traditional approach for the study of the nonequilibrium flow is to include higher-order derivatives of the macroscopic flow variables in the governing equations, such as the Burnett equations. However, in the current approach, we are undertaking an opposite path. For example, the shear stress (first-

FIG. 4. Pressure distributions in the cross stream direction for the pressure driven Poiseuille flow at $\text{Kn}=0.1$.

order spatial derivative) in the NS equation is even replaced by an algebraic temperature relaxation term (zeroth-order of spatial derivative).³

(3) The GBGK model provides a general framework to simulate the physical processes in the nonequilibrium flow regime. One of the advantages is the separation of the multiscale physics into subprocesses with different relaxation times. We can construct even more middle states between f and f^e , such as including individual quantum energy levels in g for a molecule in the study of the molecule dissociation.

(4) The GBGK model theoretically generalizes the NS constitutive relationship for the nonequilibrium flow. First, the isotropic pressure term is replaced by the multiple pressure tensor related to the multiple translational temperature. Second, the shear stress is replaced by the translational temperature relaxation. Third, the bulk viscosity term is replaced by the translational and rotational temperature relaxation. Fourth, the viscosity coefficient is generalized to $\tau \cdot p$. Fifth, we can further include nontraditional terms in the NS constitutive relations, such as the terms related to the vibrational energy relaxation and electron ionization process.

The GBGK model presented in this paper basically provides a new framework to derive macroscopic governing equations for the flows in the near continuum regime. The success of its application in the nonequilibrium flows is due to the extension of the temperature concept from a scalar to a tensor, which is directly used in the construction of the nonequilibrium gas distribution function, and due to the gas-kinetic scheme to approximate the local numerical solution.

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- ¹K. Xu, "Regularization of the Chapman–Enskog expansion and its description of shock structure," *Phys. Fluids* **14**, L17 (2002).
- ²K. Xu and E. Josyula, "Continuum formulation for nonequilibrium shock structure calculation," *Comm. Comp. Phys.* **1**, 425 (2006).
- ³K. Xu, H. Liu, and J. Jiang, "Multiple temperature kinetic model for continuum and near continuum flows," *Phys. Fluids* **19**, 016101 (2007).
- ⁴P. L. Bhatnagar, E. P. Gross, and M. Krook, "A model for collision processes in gases I: Small amplitude processes in charged and neutral one-component systems," *Phys. Rev.* **94**, 511 (1954).
- ⁵S. Chapman and T. G. Cowling, *The Mathematical Theory of Nonuniform Gases* (Cambridge University Press, Cambridge, 1990).
- ⁶T. Ohwada and K. Xu, "The kinetic scheme for full Burnett equations," *J. Comput. Phys.* **201**, 315 (2004).
- ⁷C. Park, *Nonequilibrium Hypersonic Aerothermodynamics* (Wiley, New York, 1990).
- ⁸G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows* (Oxford Science, New York, 1994).
- ⁹K. Xu, "A gas-kinetic BGK scheme for the Navier–Stokes equations and its connection with artificial dissipation and Godunov method," *J. Comput. Phys.* **171**, 289 (2001).
- ¹⁰H. Alsmeyer, "Density profiles in argon and nitrogen shock waves measured by the absorption of an electron beam," *J. Fluid Mech.* **74**, 497 (1976).
- ¹¹Y. Zheng, A. L. Garcia, and B. J. Alder, "Comparison of kinetic theory and hydrodynamics for Poiseuille flow," *J. Stat. Phys.* **109**, 495 (2002).
- ¹²M. Tij and A. Santos, "Perturbation analysis of a stationary nonequilibrium flow generated by an external force," *J. Stat. Phys.* **76**, 1399 (1994).
- ¹³M. M. Malek, F. Baras, and A. L. Garcia, "On the validity of hydrodynamics in plane Poiseuille flows," *Physica A* **240**, 255 (1997).
- ¹⁴F. J. Uribe and A. L. Garcia, "Burnett description for plane Poiseuille flow," *Phys. Rev. E* **60**, 4063 (1999).
- ¹⁵S. Hess and M. Malek-Mansour, "Temperature profile of a dilute gas undergoing a plane Poiseuille flow," *Physica A* **272**, 481 (1999).
- ¹⁶K. Aoki, S. Takata, and T. Nakanishi, "Poiseuille-type flow of a rarefied gas between two parallel plates driven by a uniform external force," *Phys. Rev. E* **65**, 026315 (2002).