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Multiple Temperature Model for Near Continuum Flows

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Abstract

In the near continuum flow regime, the flow may have different translational temperatures in different directions. It is well known that for increasingly rarefied flow fields, the predictions from continuum formulation, such as the Navier-Stokes equations, lose accuracy. These inaccuracies may be partially due to the single temperature assumption in the Navier-Stokes equations. Here, based on the gas-kinetic Bhatnagar-Gross-Krook (BGK) equation, a multi-translational temperature model is proposed and used in the flow calculations. In order to fix all three translational temperatures, two constraints are additionally proposed to model the energy exchange in different directions. Based on the multiple temperature assumption, the Navier-Stokes relation between the stress and strain is replaced by the temperature relaxation term, and the Navier-Stokes assumption is recovered only in the limiting case when the flow is close to the equilibrium with the same temperature in different directions. In order to validate the current model, both the Couette and Poiseuille flows are studied in the transition flow regime.

Keywords: Gas-kinetic model; Multiple translational temperatures; Rarefied flow

1. Introduction

The transport phenomena, i.e., mass, heat, and momentum transfer, in different flow regime is of a great scientific and practical interest. The classification of various flow regimes are based on the dimensionless parameter, i.e., the Knudsen number, which is a measure of the degree of rarefaction of the medium. The Knudsen number Kn is defined as the ratio of the mean free path to a characteristic length scale of the system. In the continuum flow regime where $Kn < 0.001$, the Navier-Stokes equations with linear relations between stress and strain and the Fourier's law for heat conduction are adequate to model the fluid behavior. For flows in the continuum-transition regime ($0.1 < Kn < 1$), the Navier-Stokes equations are known to be inadequate Zheng et al. (2002b). This regime is important for many practical engineering problems, such as the simulation of microscale flows and hypersonic flow around space vehicles in low earth orbit. Hence, there is a strong desire and requirement for accurate models which give reliable solutions with lower computational costs.

Currently, the Direct Simulation Monte Carlo (DSMC) method is the most successful technique in the numerical prediction of low density flows Bird (1994). However, in the continuum-transition regime, especially for micro-channel flows, the DSMC suffers from statistical noise in the bulk velocity because of the random molecular motion. When the bulk velocity is much slower than the thermal velocity, many independent samples are needed to eliminate the statistical scattering, as for the micro-electro-mechanical system (MEMS) simulation. In fact, for the nitrogen gas at room temperature, the standard deviation in the molecular speed is about 300 m/s Fan and Shen (2001), which would require approximately

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9 million independent samples in DSMC to reduce the scatter in the bulk velocity to 0.1 m/s. For MEMS gas flows that operate in the mm/s range, the number of required samples can grow into trillions. So, DSMC is impractical in these cases. Alternatively, many macroscopic continuum models have been intensively developed and reported in the literature. These include the Navier-Stokes and the Burnett equations from the Chapman-Enskog expansion, Grad's 13 moment equations, the regularized 13 equations, and many others Zheng et al. (2006). In order to assess these continuum models, a few test cases have been used. It seems that none of the models is commonly acceptable for rarefied flow simulations. Also, in all above models, a single translational temperature is usually assumed. Overall, the small length scales and slow bulk gas velocity combine to make continuum solutions inaccurate, and particle solution time consuming. Besides DSMC and continuum models, many alternative approaches have also been proposed in recent years, such as the empirical slip and viscosity model McNenly (2005), the information preservation (IP) method (Fan and Shen, 2001; Sun and Boyd, 2002), and the Lattice Boltzmann Method (LBM) Toschi and Succi (2005). However, IP and LBM are mostly used for the isothermal flows. More references about the methods for the microflows, such as the LBM, can be found in Karniadakis and Beskok (2002). Recently, based on the BGK model and the generalization of particle collision time for the translational non-equilibrium, a multi-scale method has been successfully developed for the argon and nitrogen shock structures for a wide range of Mach numbers, i.e., $1.2 \le M \le 11$. The current study is a continuation of the research on the rarefied gas flow using the gas-kinetic method. The objective is to provide a reliable and efficient numerical scheme in the low transition flow regime, which could be used as an alternative to the DSMC method.

The goal of this study is to construct a multiple translational temperature model. After constructing the model, the corresponding numerical scheme will be developed and applied to near continuum flow computation, such as the Couette and Poiseuille flows. n this paper, Sec. 2 provides details on the construction of the kinetic equation and Sec. 3 is about the numerical scheme to solve this model. Section 4 is about the application of the current model. The numerical solutions from the current model are compared with the DSMC results in the transition flow regime. The final section is the conclusion.

2. Multiple translational temperature kinetic model

The Boltzmann equation expresses the behavior of a many-particle kinetic system in terms of the evolution equation for a single particle gas dis-tribution function. The simplification of the Boltzmann equation given by the BGK model is formulated as bhatnagar (1954),

$$\frac{\partial f}{\partial t} + \vec{u} \cdot \frac{\partial f}{\partial \vec{x}} = \frac{f^{eq} - f}{\tau} \tag{1}$$

where f is the number density of molecules at position $\vec{x}$ and particle velocity $\vec{u} = (u, v, w)$ at time t . The left hand side of the above equation represents the free streaming of molecules in space, and the right side denotes the collision term. In the BGK model, the collision operator involves simple relaxation to a state of local equilibrium given by f^{eq} with a characteristic time scale τ . Traditionally, the equilibrium state is given by a Maxwellian,

$$f^{eq} = \rho \left(\frac{\lambda}{\pi} \right)^{\frac{K+3}{2}} e^{-\lambda((\vec{u}-\vec{U})^2 + \xi^2)}, \tag{2}$$

where ρ is the density, $\vec{U}$ the macroscopic fluid velocity, and $\lambda = \frac{m}{2kT}$. Here, m is the molecular mass, k is the Boltzmann constant, and T is the temperature. For an equilibrium flow, the internal variable ξ accounts for the rotational and vibrational modes, such as $\xi^2 = \xi_1^2 + \xi_2^2 + \cdots + \xi_K^2$, and the total number of degrees of freedom K is related to the specific heat ratio γ . In the current paper, we only consider monatomic gas with $K = 0$. Based on the above BGK model, the Navier-Stokes equations can be derived with the Chapman-Enskog expansion truncated to the 1st-order Ohwada and Xu (2004).

Traditionally, the BGK model is considered suitable only for isothermal rarefied gas flow. It does not provide reliable results for non-isothermal flows because it gives incorrect Prandtl number. The disagreement between an exact solution based on the Boltzmann equation and that obtained from the BGK model reaches 30% near the hydrodynamic flow

regime. In order to get the correct Prandtl number, many modifications of the BGK model have been proposed. One is the Ellipsoid-Statistical BGK (ES-BGK) model of Holway (1966), and the other is the S model of Shakhov Shakhov (1968). In the ES-BGK model, the "temperature" becomes a tensor and it is related to Prandtl number. In the S-model, a heat flux term is added in the equilibrium state. In our early BGK scheme for the continuum flow computation Xu (2001), the correct Prandtl number is achieved th-rough the modification of heat flux across a cell interface in a finite volume scheme. In the following, we are going to propose a multi-temperature model. The purpose of constructing this model is not for the Prandtl number correction, but for the capture of physical multi-translational temperature phenomena in the near continuum flow regime, where the accuracy of the NS equations is not adequate.

This paper mainly concerns the 2D flow simulation. In the following, a multi-T model in 2D will be proposed. The generalized BGK model has the same form as the original one,

$$\frac{\partial f}{\partial t}+u\frac{\partial f}{\partial x}+v\frac{\partial f}{\partial y}=\frac{g-f}{\tau}, \tag{3}$$

but the equilibrium state has multiple temperature,

$$g=\rho\left(\frac{\lambda_x}{\pi}\right)^{1/2}\left(\frac{\lambda_y}{\pi}\right)^{1/2}\left(\frac{\lambda_z}{\pi}\right)^{1/2} \exp[-\lambda_x(u-U)^2-\lambda_y(v-V)^2-\lambda_z w^2] \tag{4}$$

Here $\lambda_x=m/(2kT_x)$, $\lambda_y=m/(2kT_y)$, $\lambda_z=m/(2kT_z)$ and are related to the translational temperature T_x , T_y , and T_z in x-, y- and z-directions. In order to determine all unknowns in the corresponding macroscopic variables, such as ρ,U,V,T_x,T_y and T_z , we propose the following moments for the collision term in the BGK model,

$$\begin{aligned}&\int\phi\left(\frac{\partial f}{\partial t}+u\frac{\partial f}{\partial x}+v\frac{\partial f}{\partial y}\right)dudvdw\\&=\int\phi\frac{g-f}{\tau}dudvdw\\&=(0,0,0,0,\rho(E_x^{eq}-E_x)/\tau,\rho(E_y^{eq}-E_y)/\tau)^T\end{aligned} \tag{5}$$

where $\phi=[1,u,v,(u^2+v^2+w^2)/2,u^2/2,v^2/2]^T$. The 1st four moments on the right hand side of the above equation are the conservative moments of the mass, momentum, and total energy. The last two moments are the newly constructed models which simulate the energy exchange among different directions. This relaxation model for the non-conservative moments are similar to the Teller-Landau relaxation model for the energy exchange between translational and rotational degree of freedom. Since the translational energies are exchanged in different directions through particle collisions, a single relaxation time, i.e., the particle collision time, is assumed for the energy relaxation. The equilibrium energies ρE_x^{eq} and ρE_y^{eq} have the forms

$$\rho E_x^{eq}=\frac{1}{2}\rho U^2+\frac{\rho}{4\lambda^{eq}} \quad \text{and} \quad \rho E_y^{eq}=\frac{1}{2}\rho V^2+\frac{\rho}{4\lambda^{eq}} \tag{6}$$

which are obtained based on the assumption that the system will approach to an equilibrium state with equal temperature. The common equilibrium tem-perature in all directions λ^{eq} is determined by equally distributing thermal energy in all degrees of freedom,

$$\rho\frac{3}{4\lambda^{eq}}=\rho E-\frac{1}{2}\rho(U^2+V^2) \tag{7}$$

where ρE is the total energy, i.e.,

$$\begin{aligned}\rho E&=\int\frac{1}{2}(u^2+v^2+w^2)f dudvdw\\&=\int\frac{1}{2}(u^2+v^2+w^2)g dudvdw\end{aligned} \tag{8}$$

Note that the last two moments on the right hand side of Eq. (5) cannot be derived directly from the BGK Eq. (3) itself. It is a model we construct. The basic consideration is that there needs particle collision to exchange energy in different directions. The direct moments $(u^2/2,v^2/2)$ to the BGK Eq. (3) with the multiple temperature equilibrium state g in Eq. (4) will give

$$[\rho(\frac{1}{2}U^2+\frac{1}{4\lambda_x})-\rho E_x]/\tau \quad \text{and}$$
$$[\rho(\frac{1}{2}V^2+\frac{1}{4\lambda_y})-\rho E_y]/\tau\,, \tag{9}$$

for the two terms on the right hand side of Eq. (5), which are not adequate to close the system. In other

words, when we introduce the multiple temperature equilibrium state in Eq. (5), we introduce two more unknowns: λ_y and λ_z. In order to close the system to have a unique solution, we have to introduce additional two more equations or constraints, which are the last two moments in (5), where λ^{eq} can be explicitly determined through the total thermal energy in the system. So, our current multi-T BGK model is an extension of the original BGK model and the nonconservative moments are modeled instead of being directly derived from the BGK collision term. Only through the new collision moments (5), the corresponding equations are closed and the macroscopic mass, momentum, total energy, and individual energy in each direction can be updated. In Sec. 3, we are going to present the numerical method based on Eqs. (3) and (5) for the time evolution of macroscopic physical quantities. The idea in our current model is that the thermal equilibrium between x-, y-, and z-directions will be achieved through the particle collisions, and there is a time delay to achieve the temperature equilibrium. In the Navier-Stokes equations, it is assumed that the same equilibrium temperature is obtained instantaneously.

3. Finite volume scheme for multi-T kinetic model

The kinetic model constructed in the previous section is solved based on the gas-kinetic BGK scheme Xu (2001). It is a conservative multi-scale finite volume method, where the update of the macroscopic flow variables is through the numerical fluxes at cell interfaces which are evaluated based on the time-dependent gas distribution function. Since we are going to develop a directional splitting method to solve Eq. (5), the kinetic model in x-direction can be written as,

$$f_t + uf_x = (g - f)/\tau \tag{10}$$

where g is the multiple temperature equilibrium state (4). Taking moments ϕ to the above equations in a control volume $x \in [x_{j-1/2}, x_{j+1/2}]$ and time interval $t \in [t^n, t^{n+1}]$, the update of the macroscopic flow variables, i.e., $W = (\rho, \rho U, \rho V, \rho E, \rho E_x, \rho E_y)^T$ inside each numerical cell $[x_{j-1/2}, x_{j+1/2}]$ from time step t^n to t^{n+1} becomes

$$W_j^{n+1} = W_j^n + \frac{1}{\Delta x}\int_{t^n}^{t^{n+1}} (F_{j-1/2}(t) - F_{j+1/2}(t))dt + S_j^n \Delta t \tag{11}$$

where $F_{j+1/2}$ is the corresponding fluxes at a cell interface, which are evaluated based on the gas distribution function $f_{j+1/2}$ there,

$$F = \int u\phi f_{j+1/2} dudvdw . \tag{12}$$

The source term is due to the moments of the collision term in Eq. (5). For the current multi-T model, the evaluation of the gas distribution function f at a cell interface is similar to the BGK-NS method in Xu (2001), where the only difference between them is that three temperatures T_x, T_y, and T_z have to be accounted for.

After the determination of f at a cell interface, we can explicitly evaluate the heat flux there as well. 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 Xu (2001), is also implemented in the present study. Therefore, the current model can simulate flow with any Prandtl number. Due to different translational temperatures, the heat conduction term, i.e., $(5R/2)\mu\nabla T$ in the standard Navier-Stokes equations, becomes approximately $(3R/2)\mu\nabla T^{//}$ in the flow parallel direction and $(R/2)\mu\nabla T^{\perp}$ in the perpendicular direction. Therefore, there is standard meaning of Prandtl number anymore. The use of a scalar Prandtl number in the current study is basically to proportionally modify the heat flux in different directions with a scale $(1/\mathrm{Pr} - 1)$.

4. Numerical experiments

4.1 Shear driven couette flows

Shear driven Couette flows are encountered in micromotors, comb mechanisms, and microbearings. In the simplest case, the Couette flow can be used as a prototype flow to model such flows driven by a moving plate. Since the Couette flow is shear driven, the pressure does not change in the stream-wise direction. Hence, the compressibility effects become important for large temperature fluctuations or at high speeds. In this section, we simulate the Couette flows in both continuum and near continuum flow regime.

This is a gas flow problem between two infinite parallel plates, separately by a distance L. In our computation, the most cases we study are the hard sphere (HS) molecule and the working gas is argon. The specific heat ratio is $\gamma = 5/3$ with molecular mass $m = 6.63 \times 10^{-26} kg$. The viscosity coefficient

for HS is $\mu = 2.117\times10^{-5}\sqrt{T/273}N\cdot s/m^2$. The mean free path is defined as

$$l_0 = \frac{16}{5}\left(\frac{1}{2\pi RT}\right)^{1/2}\frac{\mu}{\rho_0}, \tag{13}$$

where R is the gas constant, T and ρ are temperature and density, respectively. In most calculations, both surfaces maintain room temperature *273 K* and Maxwell diffusive kinetic reflection boundary condition Xu (2001) is used. The density ρ_0 has a value corresponding to the pressure of 1atm (or *101325Pa*) at *T=273 K*. The Knudsen number is defined as l_0/L, which increases as the length L decreases. In all computations, we use 50 cells in the one-dimensional computational domain.

In the following, we simulate the Couette flow cases for the hard sphere (HS) molecules with fixed upper wall velocity *300m/s*. The use of this wall velocity is from the consideration of two folds. One is the easy solution from DSMC simulation and the other is the temperature deviation due to large shear. The Prandtl number used is *Pr=0.68*, which is consistent with the Prandtl number in the DSMC method for the HS model. The Kundsen numbers simulated are *Kn=0.01* and *0.1*. Figure 1 shows the velocity and temperature profiles across the channel at *Kn=0.01*, note three temperatures are plotted for both DSMC and multi-T solutions, even though they are indistinguishable. As the Knudsen number increases to *0.1*, the three temperatures can be clearly observed in Fig. 2, where both velocity and temperature from multi-T model have a fair agreement with the DSMC results. At this Knudsen number, the velocity profile is not a straight line. The slight curvature near the wall may be due to the Knusden layer in the DSMC solution. In terms of computational efficiency, the multi-T model takes minutes in a PC in these cases to get a steady state solution. Even though we concentrate on the HS molecules in the above simulation, the multi-T model itself can be applied to any molecular model with a generalized viscosity coefficient, such as the Sutherland's law.

4.2 External force driven poiseuille flow

It is generally recognized that in the slip flow regime with Knudsen number $Kn \le 0.1$, the Navier-Stokes equations with the slip boundary condition is capable to accurately simulate the microchannel flow.

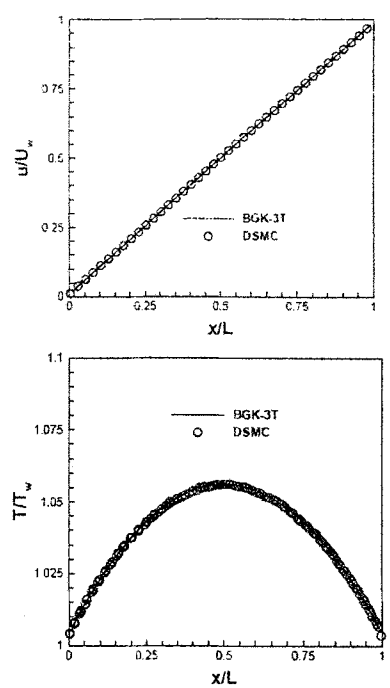

Fig. 1. Velocity and temperature distributions in Couette flow, $\mu \sim \sqrt{T}$, $Kn = 0.01$.

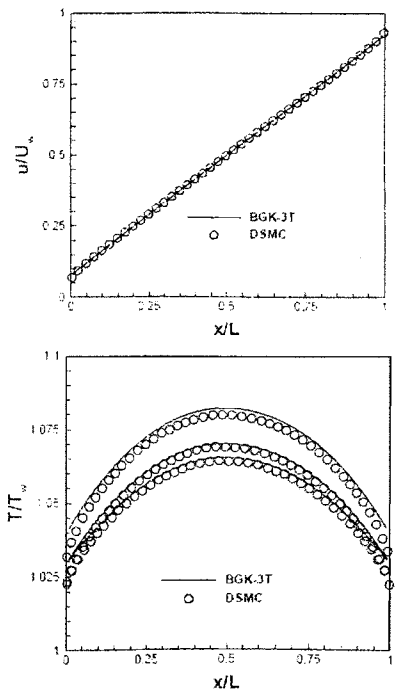

Fig. 2. Velocity and temperature distributions in Couette flow, $\mu \sim \sqrt{T}$, $Kn = 0.1$. In terms of the temperature on the right figure, the up one is T_y in the cross stream direction, the middle one is T_z , and the low one is T_x in the gas moving direction.

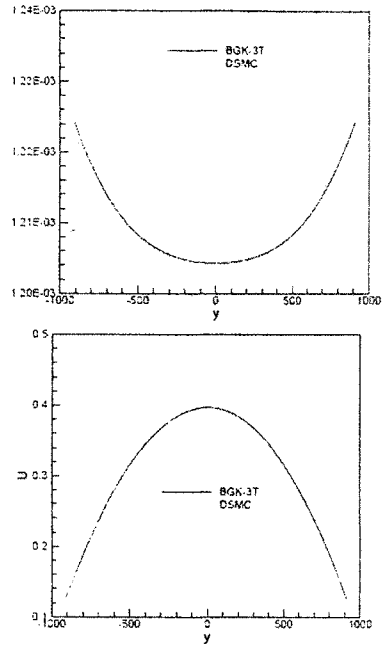

Fig. 3. Density and velocity distributions in Poiseuille flow, BGK-3T model, $Kn = 0.1$.

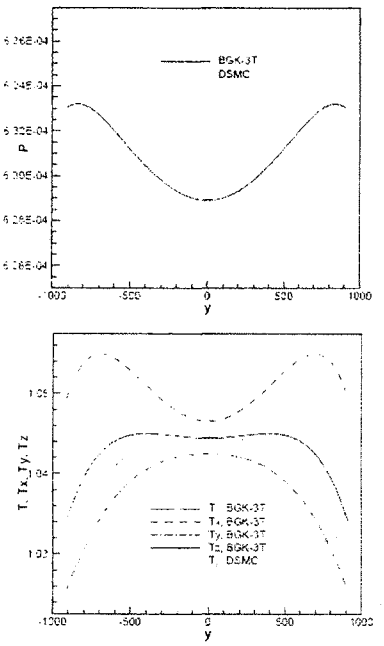

Fig. 4. Pressure and temperature distributions in Poiseuille flow, BGK-3T model, $Kn = 0.1$.

However, for the simple force driven Poiseuille flow in the slip flow regime with relatively small gradient and Knudsen number, the Navier-Stokes equations give qualitatively incorrect predictions Zheng (2002a; 2002b). For example, they fail to reproduce the central minimum in the temperature profile and non constant pressure profile, which are both predicted by the kinetic theory and observed in the DSMC simulations (Tij and Santos, 1994; Malek et al., 1997; Uribe and Garcia, 1999; Hess and Malek-Mansour, 1999; Aoki et al., 2002). In order to understand these phenomena, many analysis have been done. For example, the non-constant pressure is well explained based on the Burnett equations Uribe and Garcia (1999), and the temperature minimum at the center is explained only through the kinetic theory (Tij and Santos, 1994; Malek et al., 1997; Aoki et al., 2002), or the super-Burnett solution Xu (2003). As an excellent test for capturing non-equilibrium phenomena, the current multi-temperature model will be used to study the Poiseuille flow at $Kn=0.1$ as well.

The set up of external force driven Poiseuille flow case is the same as that given in Zheng (2002a). Figures 3 and 4 present the results from the current multi-T model. Besides the excellent match of density and velocity between the DSMC and the multi-T results, the curved pressure distribution and temperature are well captured as well. The temperature minimum in both T_x and the averaged temperature T can be clearly observed in Fig. 4. This is surprising because the analysis in Uribe and Garcia (1999) confirms that the temperature minimum does not appear even in the Burnett solution. But, it can be recovered in the super-Burnett order Xu (2003). However, based on our current model, the temperature minimun has been recovered. So, the use of temperature relaxation in multi-T model to replace the stress and strain relation in the Navier-Stokes equation has significant impact in capturing the non-equilibrium physical phenomena in the near continuum flow regime.

5. Conclusion

In this paper, a gas-kinetic model for the multi-translational temperature is proposed and applied to the near continuum flow computation. Based on the successful application of the current model, it becomes evident that besides modeling slip boundary condition as discussed in the literature Kamiadakis and Beskok (2002), the multiple temperature effect has to be considered as well for the near continuum flow. The current kinetic model and its numerical method provide an effective tool for the study of

micro-flows in the near continuum flow regime, where the DSMC method can be very expensive. Theoretically, the DSMC method is an operator splitting method with decoupling particle transport and collision. It requires that the numerical time step is smaller than the particle collision time, which cannot be tolerated in the continuum flow regime, especially for high Reynolds number flows. However, in the continuum flow regime with a single translational temperature assumption the current multi-temperature numerical scheme will go back to the BGK-NS method, which is an accurate compressible Navier-Stokes flow solver.

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