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Multiple temperature kinetic model and its applications to micro-scale gas flows

Hongwei Liu [a,*], Kun Xu [b], Taishan Zhu [c], Wenjing Ye [c]

[a] State Key Laboratory of High Temperature Gas Dynamics, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, China
[b] Department of Mathematics, The Hong Kong University of Science and Technology, Kowloon, Hong Kong
[c] Department of Mechanical Engineering, The Hong Kong University of Science and Technology, Kowloon, Hong Kong

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ABSTRACT

This paper presents a gas-kinetic scheme to solve the multiple temperature kinetic model (MTKM), which was proposed in J. Comput. Math. 29(6) (2011) 639–660, for the study of non-equilibrium flows. The MTKM is a two-stage particle collision model possessing an intermediate quasi-equilibrium state with a symmetric second-order temperature tensor. A gas-kinetic finite volume scheme is developed for the numerical solution of the MTKM in the continuum and transition flow regimes. The gas-kinetic scheme is designed for the updating of macroscopic variables, which include the conservative flow variables and the multiple temperature field. In order to validate the kinetic model, the gas-kinetic scheme is used in the study of lid-driven cavity flows in both continuum and transition flow regimes. The numerical results predicted by the MTKM are compared with those from the direct simulation Monte Carlo (DSMC) method, the Navier–Stokes equations (NSE), and the early three-temperature kinetic model (TTKM) proposed in Phys. Fluids 19, 016101(2007). It is demonstrated that the MTKM has obvious advantages in comparison with the NSE and the TTKM in capturing the non-equilibrium flow behavior in the transition flow regime. One distinguishable phenomenon captured by the MTKM is that in the transition flow regime the heat flux direction can be from a low temperature to a high temperature region, which violates the Fourier's law of continuum flows. The MTKM provides a more accurate physical model than the NSE for the non-equilibrium flows.

1. Introduction

Gas flows can be categorized into different flow regimes based on the Knudsen number Kn. In the continuum regime ($Kn < 0.001$), the Navier–Stokes equations (NSE) are adequate to model the fluid behavior. In the near continuum regime ($0.001 < Kn < 1$), the NSE are known to lose accuracy or be inadequate. In fact this regime is encountered in many practical engineering problems, for example those in aerospace engineering and Micro-Electro-Mechanical Systems (MEMS). Therefore, how to realize reliable numerical simulations of gas flows in this regime at low computational costs are of great interest from both scientific and practical views.

Currently the direct simulation Monte Carlo (DSMC) method is one of the most successful techniques for the non-equilibrium gas flows. However, the DSMC becomes very inefficient for near continuum and low speed flows because of the cell size restriction and the statistical noise. Various modifications have been proposed in order to improve the efficiency of the standard DSMC, for example the information preservation (IP) method [3–6], the variance reduction approach [7], the low Mach number DSMC algorithm [8] and the hybrid methods [9,10], just to name a few. Alternative methods, which directly solve the Boltzmann or model equations [11–15], have also attracted increasing attentions recently.

One of the continuum-based approaches in modeling the non-equilibrium flows is to use the high order governing equations derived from the Bhatnagar–Gross–Krook (BGK) model by the Chapman-Enskog expansion, for instance the Burnett and super-Burnett equations. However, it has been well recognized that these equations have the stability problems and cannot be directly used in numerical simulations [16]. In recent years, some improvements have been proposed in order to cure these problems [17–19]. Another strategy for non-equilibrium flow simulations is deriving various governing equations by the moment closure technique, such as Grad's 13 moment equations [20], the regularized 13 (R13) and 26 (R26) moment equations [21,22], Levermore's 10 moment system [23], and many others.

Recently, a multiple temperature kinetic model (MTKM) was proposed [1] for continuum and near continuum flow simulations, which is a nature extension of an early kinetic model [2,24]. The main difference between the two kinetic models is that the former defines the translational temperature as a second-order symmetric tensor while the latter only uses three translational temperatures in the x-, y- and z-directions. This is the reason that the latter is

* Corresponding author. Tel.: +86 10 82544022; fax: +86 10 62561284.
E-mail address: hliu@imech.ac.cn (H. Liu).

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renamed the three-temperature kinetic model (TTKM) here. In fact, prior to these two models, the gas-kinetic schemes describing the non-equilibrium flows related to the molecular rotational and vibrational degrees of freedom have been introduced for the shock structure calculations [25,26], where three different temperatures, i.e. the translational, rotational and vibrational temperatures, are used for modeling the non-equilibrium effects.

In [1], the generalized macroscopic gas dynamic equations based on the MTKM have been derived and analyzed, some quasi-one-dimensional numerical tests have been shown to demonstrate the performance of the MTKM in the micro-scale flow simulations. In the present work, instead of solving the corresponding macroscopic equations, a gas-kinetic scheme will be developed for the MTKM directly, and some truly two-dimensional (2D) test cases for the micro-scale gas flows will be presented in order to evaluate the capability of the MTKM in modeling the non-equilibrium flows.

2. Multiple temperature kinetic model and the gas-kinetic scheme

In this section, we briefly review the essentials of the MTKM and propose a finite volume gas-kinetic scheme as well as the wall boundary condition to get the numerical solutions of the MTKM.

2.1. A brief review of the MTKM

The three-temperature kinetic model for continuum and near continuum flows was proposed in [2], where only three translational temperatures for monotonic gases are used in the construction of the model. Numerical tests [2,24] have demonstrated some success of the TTKM in describing the non-equilibrium gas flows. However, the defects of the early model are also obvious: the applications of the model in numerical simulations will depend on the choice of the coordinate system, since only three translational temperatures in the x-, y- and z-directions are considered. Theoretically from the extended definition of temperature it should be a second-order symmetric tensor, in that case the model's utility will be independent of the coordinate system used.

These problems were cured in [1], where the temperature is defined as a second-order symmetric tensor and used to construct an improved gas-kinetic model, i.e. MTKM, for non-equilibrium flow simulations. The two-stage MTKM can be written as [1]

$$\frac{\partial f}{\partial t}+\mathbf{u}\cdot\nabla f=\frac{g-f}{\tau}+Q, \tag{1}$$

where t is the time, $\mathbf{u}=(u,v,w)$ is the velocity of the gas particle, τ is the collision time representing the relaxation rate of the distribution function f due to the collisions, $Q=(f^{eq}-g)/\tau$, which is treated as a special source term different from the term $(g-f)/\tau$ in the model [1], therefore, although this model is identical to the BGK model mathematically, the physical significance of two models is different. In the MTKM, the whole relaxation process of the non-equilibrium distribution function f to the Maxwellian equilibrium state f^{eq} is separated into two sub-processes: (i) f relaxes to an intermediate state g between f and f^{eq}; (ii) the intermediate distribution g relaxes to the Maxwellian equilibrium state f^{eq}. Although other choices may be possible, in our study the intermediate state g is assumed to be a Gaussian distribution

$$g=\frac{\rho}{\sqrt{\det(2\pi R\mathbf{T})}}\exp\left[-\frac{1}{2}(\mathbf{u}-\mathbf{U})(R\mathbf{T})^{-1}(\mathbf{u}-\mathbf{U})^{\mathrm{T}}\right], \tag{2}$$

where ρ is the density, R is the gas constant, $\mathbf{U}=(U,V,W)$ is the macroscopic velocity of the gas, $\mathbf{T}$ is the symmetric second-order temperature tensor, and for monatomic gas it reads

$$\mathbf{T}=\begin{pmatrix}T_{xx} & T_{xy} & T_{xz}\\ T_{xy} & T_{yy} & T_{yz}\\ T_{xz} & T_{yz} & T_{zz}\end{pmatrix}.$$

By taking moments $\Psi=(1,u_i,u_iu_j/2)^{\mathrm{T}}$ of Eq. (1) and using the Chapman-Enskog or iterative expansion, the following generalized gas dynamic (GGD) equations based on the MTKM can be derived [1],

$$\partial_t\rho+\partial_k(\rho U_k)=0, \tag{3}$$

$$\partial_t(\rho U_i)+\partial_k[\rho(U_iU_k+RT_{ik})]=\partial_k[\rho R(\overline{T}\delta_{ki}-T_{ki})], \tag{4}$$

$$\begin{aligned}&\partial_t[\rho(U_iU_j+RT_{ij})]+\partial_k[\rho(U_iU_jU_k+RU_kT_{ij}+RU_iT_{jk}+RU_jT_{ki})]\\&=\frac{2}{\tau}\rho R(\overline{T}\delta_{ij}-T_{ij})+\partial_k\{\rho R[U_k(\overline{T}\delta_{ij}-T_{ij})+U_i(\overline{T}\delta_{jk}-T_{jk})\\&\quad+U_j(\overline{T}\delta_{ki}-T_{ki})]\}-\partial_kQ_{ijk},\end{aligned} \tag{5}$$

where δ_{ij} is the Kronecker delta function, the averaged temperature $\overline{T}$ is obtained by

$$\overline{T}=\frac{1}{3}\sum_{l=1}^{3}T_{ll}, \tag{6}$$

and $\mathbf{Q}$ is the generalized heat flux given by

$$Q_{ijk}=-\frac{\tau\rho R^2}{\mathrm{Pr}}(T_{kl}\partial_lT_{ij}+T_{il}\partial_lT_{jk}+T_{jl}\partial_lT_{ki}), \tag{7}$$

where Pr is the Prandtl number.

Moreover, it has been shown by theoretical analysis in [1] that the standard NSE can be recovered from the first-order GGD equations in the continuum limit ($Kn\to 0$), which will also be clearly demonstrated by our numerical examples in this paper. Interested readers may refer to [1] for the construction of the MTKM, the detailed derivation and analysis of the GGD equations based on the MTKM for non-equilibrium gas flow simulations. One point that needs to be emphasized is that the numerical method presented in the next subsection is for the MTKM directly and the GGD equations are not explicitly used in the construction of the gas-kinetic scheme.

2.2. A numerical approach to solve the MTKM

Now we present the numerical approach to solve the MTKM. The numerical method for the MTKM is a finite volume scheme, which is similar to the numerical algorithm employed in [2] for the early TTKM. Both of the two methods are extensions from the gas-kinetic BGK solver for the NSE [31]. For simplicity, the 2D cases will be considered hereafter in this paper, but the scheme presented here can be also extended to three-dimensional problems.

For 2D gas flows, we have $T_{xz},T_{yz}=0$ for the temperature tensor $\mathbf{T}$. By taking moments, the macroscopic variables are defined as

$$\mathbf{W}=\int g\Psi_{2D}dudvdw=(\rho,\rho U,\rho V,E_{xx},E_{yy},E_{zz},E_{xy})^{\mathrm{T}}, \tag{8}$$

where

$$\Psi_{2D}=(1,u,v,u^2/2,v^2/2,w^2/2,uv/2)^{\mathrm{T}}, \tag{9}$$

and

$$E_{ij}=\rho(U_iU_j+RT_{ij})/2, \tag{10}$$

with $i,j=1,2,3$ representing x,y,z, respectively. Under the finite volume framework, for a uniform grid the updating of the cell-averaged value $\mathbf{W}_{p,q}$ over the cell (p,q) from the time t^n to t^{n+1} can be obtained by

$$\mathbf{W}_{p,q}^{n+1}=\mathbf{W}_{p,q}^{n}+\frac{1}{\Delta x}\left(F^{x,\Delta t}_{p-\frac{1}{2},q}-F^{x,\Delta t}_{p+\frac{1}{2},q}\right)+\frac{1}{\Delta y}\left(F^{y,\Delta t}_{p,q-\frac{1}{2}}-F^{y,\Delta t}_{p,q+\frac{1}{2}}\right)+\mathbf{S}^{\Delta t}_{p,q}, \tag{11}$$