A multiple temperature kinetic model and its application to micro-scale gas flow simulations

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Abstract

This paper presents a numerical approach to solve the multiple temperature kinetic model (MTKM) proposed in AIAA 2009-672, then shows some applications in micro-scale gas flow simulations. The numerical results predicted by the MTKM are compared with those from Direct Simulation Monte Carlo (DSMC) method, the Navier-Stokes (NS) equations, 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 NS equations and the TTKM in study of micro-scale gas flows.

Keywords Non-equilibrium flows, kinetic model, micro-scale flows.

1. Introduction

Gas flows can be classified according to the flow regimes based on the Knudsen number. In the continuum regime (Kn<0.001), the NS equations are adequate to model the fluid behavior. In the near continuum regime (0.001<Kn<1), the NS equations are known to lose accuracy or be inadequate. This regime is encountered in many practical engineering problems, and accurate models that can give reliable solutions at low computational costs are of a great scientific and practical interest.

Currently the DSMC method is the most successful technique for low density gas flows. Various modifications have been proposed in order to improve the efficiency of the standard DSMC for low speed micro-scale gas flows, for example the well-established information preservation (IP) method[3,4,5]. One of the alternative approaches in modelling the non-equilibrium flows is that based on moment closures, such as Grad's 13 moment equations[6], the regularized 13 (R13) or 26 (R26) moment equations[7,8], Levermore's 10 moment system[9], and many others.

Recently, the MTKM was proposed[1] for near continuum flow simulations, which is the nature extension of an early kinetic model[2]. The main difference between the two approaches is that the former defines the temperature as a second-order symmetric tensor while the later only uses three temperatures in the *x*-, *y*- and *z*-directions, which is also the reason that we name the later TTKM here. In the present work, first a numerical approach is introduced to solve the MTKM, then some numerical tests for micro-scale gas flows are shown in order to evaluate the performance of the kinetic model in modelling the non-equilibrium flows.

2. Numerical approach for MTKM

The two-stage MTKM can be written as

$$f_t + \mathbf{u}\cdot\nabla f = (g - f)/\tau + Q, \qquad (1)$$

where $Q = (f^{eq} - g)/\tau$. In the MTKM, the total relaxation process of the non-equilibrium distribution f to the Maxwell equilibrium f^{eq} is separated into two sub-processes: (i) f relaxes to an intermediate state g between f and f^{eq}; (ii) g relaxes to the Maxwell equilibrium f^{eq}. The intermediate state g is assumed to be a Gaussian distribution,

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

where $\mathbf{T}$ is the temperature tensor, for monatomic gas it reads

$$\mathbf{T} = \begin{pmatrix} T_{xx} & T_{xy} & T_{xz} \\ T_{xy} & T_{yy} & T_{yz} \\ T_{xz} & T_{yz} & T_{zz} \end{pmatrix}. \qquad (3)$$

By taking moments $\psi = (1, u_i, u_i u_j/2)^{\mathrm{T}}$ of Eq. (1) and using the Chapman-Enskog or iterative expansion, we can derive the generalized gas dynamic (GGD) equations based on the MTKM. It was shown[1] that the first-order GGD equations can recover the standard NS equations in the continuum flow regime. For two-dimensional (2D) gas flow problems, we have $T_{xz} = T_{yz} = 0$. For simplicity, we describe the numerical approach to solve the MTKM for 2D problems in this paper, but the scheme is also applicable for 3D cases.

Similar to the numerical algorithm used in [2] for TTKM, the finite volume method in solving MTKM is divided into two main parts: (i) the calculation of numerical flux across cell interfaces; (ii) source term discretization. The macroscopic variables are defined as

$$\mathbf{W} = (\rho, \rho U, \rho V, E_{xx}, E_{yy}, E_{zz}, E_{xy})^{\mathrm{T}}, \qquad (4)$$

and for uniform grid the updating of the cell-averaged value $\mathbf{W}_{i,j}$ from time step t^n to t^{n+1} is obtained by

$$\mathbf{W}_{i,j}^{n+1} = \mathbf{W}_{i,j}^{n} + \frac{1}{\Delta x}(F_{i-1/2,j} - F_{i+1/2,j}) + \frac{1}{\Delta y}(F_{i,j-1/2} - F_{i,j+1/2}) + \Delta t \mathbf{S}_{i,j}^{n} \quad (5)$$

where $\mathbf{S} = (0,0,0,c(T^{eq} - T_{xx}), c(T^{eq} - T_{yy}), c(T^{eq} - T_{zz}), -cT_{xy})^{\mathrm{T}}$ with $c = 0.5\rho R/\tau$ and $T^{eq} = (T_{xx} + T_{yy} + T_{zz})/3$. For the current model, the numerical flux is obtained from the distribution function f at cell interface based on the MTKM. Specifically, we use

$$f = g - \tau(g_t + ug_x + vg_y) + tg_t, \quad (6)$$

and the relation between τ and the dynamic viscosity coefficient μ is $\tau = \mu/(\rho R T^{eq})$. We can evaluate g_x and g_y from $\mathbf{W}_x$ and $\mathbf{W}_y$ at the cell interface, respectively. Unlike those in [2], here g_x can not be explicitly determined from $\mathbf{W}_x$, therefore we first assume $g_x = g\psi_{2D}^{\mathrm{T}}\mathbf{a}$ with $\psi_{2D} = (1, u, v, u^2/2, v^2/2, w^2/2, uv/2)^{\mathrm{T}}$ and $\mathbf{a} = (a_1, a_2, a_3, a_4, a_5, a_6, a_7)^{\mathrm{T}}$, then $\mathbf{a}$ can be obtained by numerically solving the system of 7 equations

$$\int \psi_{2D} g_x du dv dw = \left(\int \psi_{2D}\psi_{2D}^{\mathrm{T}} g du dv dw\right)\mathbf{a} = \mathbf{M}\mathbf{a} = \mathbf{W}_x. \quad (7)$$

Similarly, g_y can be obtained from $\mathbf{W}_y$. After determining g_x and g_y, we may assume $g_t = g\psi_{2D}^{\mathrm{T}}\mathbf{A}$ with $\mathbf{A} = (A_1, A_2, A_3, A_4, A_5, A_6, A_7)^{\mathrm{T}}$, then **A** can be gained from

$$\int (g_t + ug_x + vg_y) du dv dw = 0. \quad (8)$$

Now the distribution function f at the cell interface is totally determined from Eq. (6), which can be used to get the numerical flux in Eq. (5). A modification of the heat flux in energy transport[2] is implemented in order to model the flow with any realistic Prandtl number. For the wall boundary, a treatment similar to that in [2] is used. The mathematical formulae for various moments of the Gaussian distribution g can be obtained by the software Mathematica.

3. Numerical tests for micro-scale gas flows

The 2D lid-driven cavity flow is used to evaluate the MTKM, which has been studied extensively[9,10]. In the present tests, the fully diffuse reflection is assumed for all the walls.

In the first case, the upper lid velocity U_w is 15.39m/s (Ma=0.05) with the upper wall temperature 273K and all other walls with temperature 546K. The Knudsen number is Kn=0.1. Fig. 1 shows the U-velocity along a vertical line crossing the cavity center, and Fig. 2 gives the V-velocity along a horizontal line crossing the center. Due to the large temperature gradient, this test case is not an easy one for many continuum-based approaches. Overall, the velocity field predicted by the MTKM is closer to that by the DSMC than those by the NS equations and the TTKM. Fig. 3(a) and Fig. 3(b) show the distributions of the temperature Txy by the DSMC and the MTKM, respectively. The agreement between the DSMC and MTKM data is good.

The second test considers the case with U_w =10m/s, Kn=0.2 and all walls with temperature 273K. In Fig. 4, a comparison of the DSMC, NS equations, TTKM and MTKM is made for the averaged temperature T and the stream traces of heat flux vector $\mathbf{q}$, which is defined as

$$q_i = \frac{1}{2}\int (u_i - U_i)(\mathbf{u} - \mathbf{U})^2 f du dv dw. \quad (9)$$

The temperature T distribution by MTKM agrees much better with that by DSMC than those by the NS equations and TTKM. As shown and discussed in [7], the very interesting thing is that the heat flow direction is from the cold to hot region under the non-equilibrium flow condition here. The NS equations and the TTKM fail to capture this counter-gradient heat flux pattern, but the MTKM can capture this unusual phenomenon very well.

The third example is about a relatively large velocity case with U_w =100m/s, Kn=0.2 and all walls with temperature 273K. The numerical results are shown in Fig. 5. Compared with the high reliable DSMC method, the NS equations can not predict the cold region around the upper left corner, the TTKM performs better than the NS equations and the MTKM can capture it well. Regarding to the hot region around the upper right corner, the results by the NS equations and MTKM are closer to the DSMC data than those by TTKM. Again, the counter-gradient heat flux phenomenon can be well captured by both the DSMC and the MTKM, but the NS equations and the TTKM are failed to cspture it.

4. Conclusions

A numerical algorithm for solving the MTKM is proposed in this paper. Instead of using the macroscopic GGD equations, the current kinetic scheme solves the MTKM to evaluate the gas distribution function at the cell interface, then calculate the numerical fluxes there by taking moments of the distribution function. The numerical procedure is similar to that of the gas-kinetic BGK solver [12] for the NS equations, and the numerical method for the TTKM [2].

The numerical tests for the micro-scale gas flows demonstrate that the MTKM has obvious advantages over the NS equations and the TTKM for modelling

the non-equilibrium flows in the near continuum regime, especially for the flows with complicated flow structures.

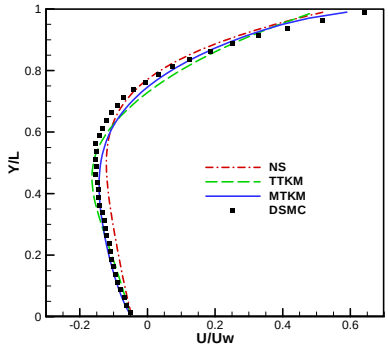


Fig. 1: The U-velocity along a vertical line crossing the cavity center.

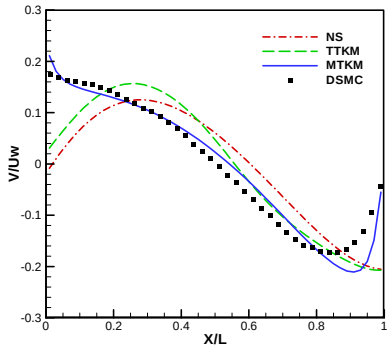
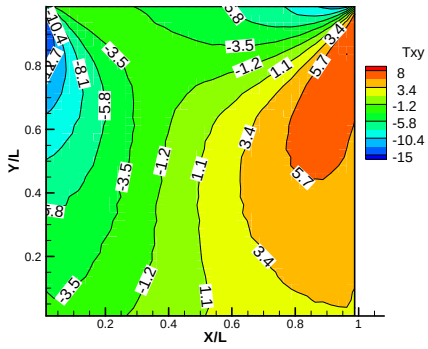
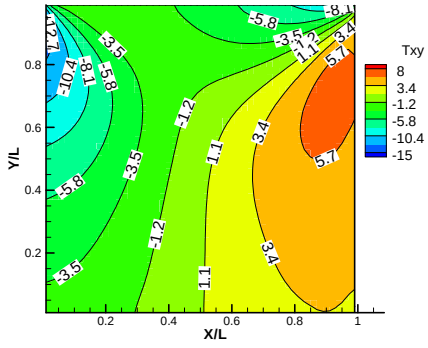


Fig. 2: The V-velocity along a horizontal line crossing the cavity center.

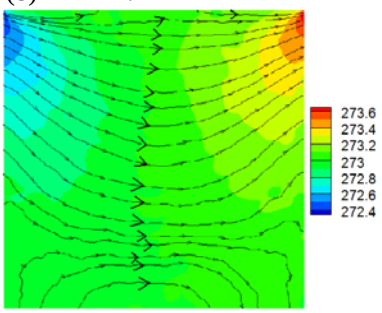


(a) DSMC

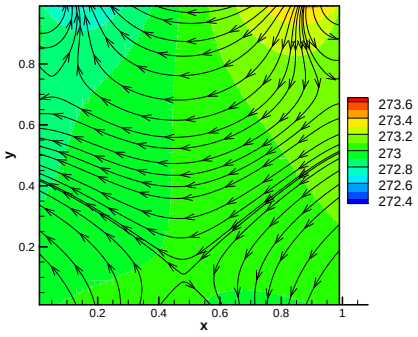


(b) MTKM

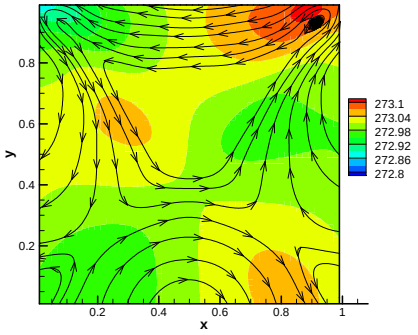
Fig. 3: The distributions of Txy predicted by: (a) DSMC and (b) MTKM.



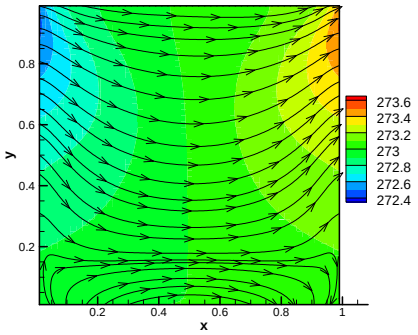
(a) DSMC



(b) NS

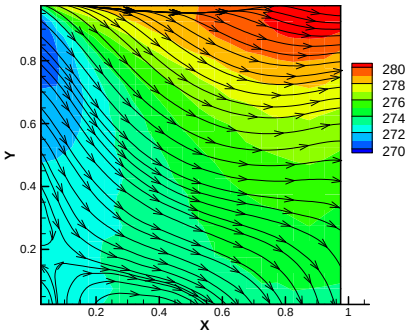


(c) TTKM

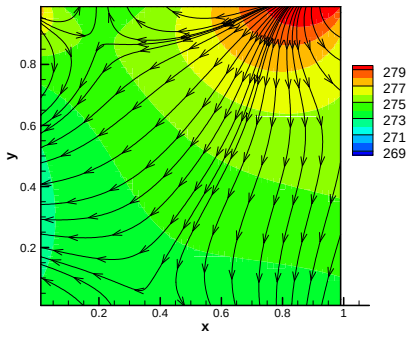


(d) MTKM

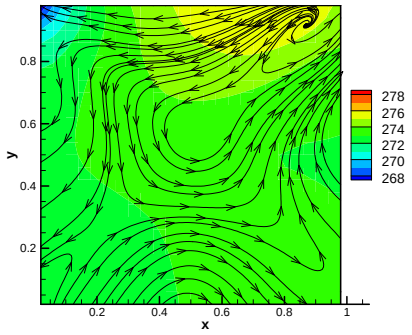
Fig. 4: Heat flux stream traces overlaid on the temperature *T* contours by: (a) DSMC, (b) NS, (c) TTKM and (d) MTKM for the case with Kn=0.2 and U_w =10m/s.



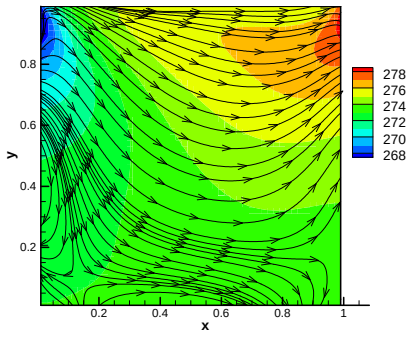
(a) DSMC



(b) NS



(c) TTKM.



(d) MTKM

Fig. 5: Heat flux stream traces overlaid on the temperature *T* contours by: (a) DSMC, (b) NS, (c) TTKM and (d) MTKM for the case with Kn=0.2 and U_w =100m/s.

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