Application of a 7-moment model with slip boundary conditions to Fourier flow

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Abstract. The solution of Kliegel's gas dynamic equations for seven moments of the velocity distribution functions that include mass, momentum, and directional temperatures, is examined for the one-dimensional heat transfer problem. The slip boundary conditions for the gas-surface interface are derived. The obtained solutions are compared to the DSMC predictions.

Keywords: Translational nonequilirbium, moment equations, slip boundary conditions
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INTRODUCTION

Anisotropy of the molecular velocity distribution function is important for rarefied gases characterized by strong thermal non-equilibrium. Such a translational anisotropy arises both in compression flows dominated by shock waves, and expanding flows such as nozzle expansions and plumes. In both cases, taking into account the translational anisotropy is critical for accurate flow modeling. The need to account for the anisotropy in nonequilibrium gases was understood as early as 1867 [1]. Besides the transitional rarefied flow regime, this anisotropy may be important in turbulent flow modeling, especially when the transition to turbulence needs to be predicted. The latter one is traditionally approached with continuum methods based on the solution of Navier-Stokes equations, which, as was pointed out in Ref. [2], may not be the correct approximate solution of the Boltzmann equation for this case.

In Ref. [2], an anisotropic fluid seven equation set was presented for the density, three fluid velocity components, and three directional thermal kinetic energies. This technique, based on a Chapman-Enskog-like expansion of the velocity distribution function over an ellipsoidal distribution function, represents a macroscopic approach to non-equilibrium flows, and as such complements microscopic, kinetic methods, in their consideration of flow nonequilibrium. In the past, several researchers have attempted to include translational non-equilibrium in a macroscopic fashion. Candler et al. [3] developed a multi-temperature equation set and compared numerical solutions for the normal shock wave problem with DSMC results. Dogra et al. [4] presented calculations using a multi-temperature model for unsteady blast-type problems. A numerical method for Maxwell's moment equations for the normal shock problem was presented in Ref. [5].

Previous study [6] has shown that the 7-moment model provides fairly accurate solutions to the shock wave problem for relatively low Mach numbers, and has some and numerical issues for hypersonic shocks. The main objective of the present work is an assessment of the accuracy of the 7-moment model predictions for surface-dominated 1D Fourier heat transfer problem in the range of Knudsen numbers where the conventional Navier-Stokes approach begins to fail. Slip boundary conditions for the 7-moment model, derived similarly to the conventional 5-moment slip conditions [7], are presented, and the results are compared with those obtained by two other approaches, solution of the Navier-Stokes equations and the DSMC method.

SEVEN MOMENT GAS DYNAMIC EQUATIONS

Similar to the conventional Euler and Navier-Stokes equations for the first five moments of the velocity distribution function f, gas dynamic equations may also be derived for seven moments of f [2], namely for gas density, velocity in three spatial directions, and three directional temperatures, which are defined as

$$T_i = \frac{1}{R}\int_{-\infty}^{\infty} c_i^2 f(\mathbf{c}) d\mathbf{c},$$

where the index i refers to spatial direction (x, y, or z), R is the gas constant, and $\mathbf{c} \equiv (c_x, c_y, c_z)$ is the thermal velocity. These equations are written as the mass, momentum, and energy conservation equations, and for the Maxwell molecule interaction model they reduce to [2]

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \tag{1}$$

$$\frac{\partial(\rho u_i)}{\partial x_i} \frac{\partial\left[\rho u_i^2 + RT_i\right]}{\partial x_i} + \frac{\partial(\rho u_i u_j)}{\partial x_j} + \frac{\partial(\rho u_i u_k)}{\partial x_k} = \frac{\partial \tau_{ij}}{\partial x_j} + \frac{\partial \tau_{ik}}{\partial x_k} \tag{2}$$

$$\frac{\partial\left[\rho u_i^2 + RT_i\right]}{\partial t} + \frac{\partial\left[\rho(u_i^3 + 3u_i RT_i + q_{iii})\right]}{\partial x_i} + \frac{\partial\left[\rho(u_i^2 u_j + u_j RT_i + q_{iij}) - 2u_i \tau_{ij}\right]}{\partial x_j} +$$
$$\frac{\partial\left[\rho(u_i^2 u_k + u_k RT_i + q_{iik}) - 2u_i \tau_{ik}\right]}{\partial x_k} = -\rho \nu (RT_i - RT) \tag{3}$$

Here, ν is the collision frequency, and indices $i \neq j \neq k$ denote any of the spatial directions x, y, and z, so equations 2 and 3 each stand for three equations for the three spatial directions. For this equation set to be closed, the shear stress

$$\tau_{ij} = \rho \int_{-\infty}^{\infty} c_i c_j f(\overline{c}) d\overline{c}$$

and heat flux

$$q_{ijk} = \frac{1}{2}\rho \int_{-\infty}^{\infty} c_i c_j c_k f(\overline{c}) d\overline{c}$$

need to be specified in terms of the above seven moments of f. Such a closure was proposed in Ref. [2] and is written as

$$\tau_{ij} = \frac{R\rho}{\nu}\left[T_j \frac{\partial u_i}{\partial x_j} + T_i \frac{\partial u_j}{\partial x_i}\right] \tag{4}$$

and

$$q_{iii} = -\frac{R^2 \rho T_i}{4\nu}\left[7\frac{\partial T_i}{\partial x_i} + \frac{\partial T_j}{\partial x_i} + \frac{\partial T_k}{\partial x_i}\right], \quad q_{ijj} = -\frac{R^2 \rho T_i}{12\nu}\left[3\frac{\partial T_i}{\partial x_i} + 5\frac{\partial T_j}{\partial x_i} + \frac{\partial T_k}{\partial x_i}\right]. \tag{5}$$

Note that the above equation set reduces to the classical Navier-Stokes equations for equal directional temperatures $T_i = T_j = T_k$. The expressions for the components of the shear stress and heat flux were validated in Ref. [6]. In that work, the shear stresses directly sampled in the DSMC method were compared to the Navier-Stokes and 7-moment values evaluated using the DSMC macroscopic properties for a 2D hypersonic flow over a sphere-cone configuration. The 7-moment approach was found to provide a significantly better agreement with the DSMC results than the Navier-Stokes relations.

SLIP BOUNDARY CONDITIONS

Application of the 7-moment equation set to model gas flow in slip regime implies that some kind of slip boundary conditions need to be set at the gas-surface interfaces in order to more accurately describe the flow. In this work, the derivation of the slip boundary conditions for directional temperatures and velocities closely follows the conventional derivation for the Navier-Stokes equations [7]. As in Ref. [7], the Maxwell model of gas-surface interactions is assumed, with the number of molecules reflected specularly and diffusely $(1-\theta)$ and θ, respectively. For this model, with known form of the velocity distribution function of molecules that come to the surface, f_s, it is possible to derive expressions for the total mass, momentum, and directional energy fluxes in the direction of the outward normal to the surface. Without loss of generality, it is assumed hereafter that the direction of the normal coincides with the positive y direction.

According to the Maxwell model, the fraction θ of all molecules colliding with the surface will fully accommodate on the surface and thus will be distributed according to f_w, where f_w is the Maxwellian distribution function with zero macroscopic velocity and a temperature equal to the surface temperature. The fraction $1-\theta$ of colliding molecules will be distributed according to $f'_s(c_x, c_y, c_z) = f_s(c_x, -c_y, c_z)$. It is therefore possible to present the total flux of some velocity-dependent property $P(\mathbf{c})$ as the sum of incoming and outcoming molecules,

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} Pu_y f_s(c_x,c_y,c_z)\,dc_x\,dc_y\,dc_z = \int_{-\infty}^{\infty}\int_{-\infty}^{0}\int_{-\infty}^{\infty} Pu_y f_s(c_x,c_y,c_z)\,dc_x\,dc_y\,dc_z +$$

$$+(1-\theta)\int_{-\infty}^{\infty}\int_{0}^{\infty}\int_{-\infty}^{\infty} Pu_y f'_s(c_x,c_y,c_z)\,dc_x\,dc_y\,dc_z + \theta\int_{-\infty}^{\infty}\int_{0}^{\infty}\int_{-\infty}^{\infty} Pu_y f_w(c_x,c_y,c_z)\,dc_x\,dc_y\,dc_z. \quad (6)$$

After that, the known form of the velocity distribution function is used in Eqn. 6 along with the specific property P. Similar to Ref. [7], the distribution function in the 7-moment equation set is presented as the following expansion in terms of the components of the thermal velocity,

$$f(\overline{c}) = f_0(\overline{c})\left(1 + a_x H_x + \ldots + \frac{1}{2}a_{xx}H_x^2 + \frac{1}{2}a_{xy}H_x H_y + \ldots + \frac{1}{6}a_{xxx}H_x^3 + \frac{1}{6}a_{xxy}H_x^2 H_y + \ldots\right), \quad (7)$$

where $f_0(\overline{c}) = \frac{n}{(2\pi R)^{3/2}\sqrt{T_x T_y T_z}} \exp\left\{-\frac{\mathbf{H}^2}{2}\right\}$ is the equilibrium distribution function, and $H_i = \frac{c_i}{\sqrt{RT_i}}$. The coefficients a that are generally functions of gas macroparameters, depend on the equation under consideration, and for the 7-moment equation set Eqs. (1)-(3) may be directly related to the coefficients used in the expansion proposed in Ref. [2],

$$f(\overline{c}) = f_0(\overline{c})\left(1 + \frac{1}{\nu}\left[A_i c_i + A_{ij} c_i c_j + A_{ijk} c_i c_j c_k\right],\right) \quad (8)$$

where the subscripts i, j, k refer to spatial directions. The exact definition of the coefficients A of Eq. (8) may be found in Ref. [2].

The expressions for the slip wall boundary conditions are calculated after substitution of gas dynamic properties (density, momentum, and directional temperatures) and the expansion (7) into Eq. 6. If the property P is density, then equation 6 reduces to

$$\rho_s\sqrt{T_{sy}} = \rho_w\sqrt{T_{wy}} \quad (9)$$

For the tangential momentum flux, simple transformations of the wall flux equations result in

$$\sqrt{RT_{sx}}\left(\frac{2-\theta}{\theta}\sqrt{\frac{\pi}{2}}a_{xy} + \frac{a_{xyy}}{2}\right) + u_x = 0 \quad (10)$$

Similar expression for the normal momentum flux may be written as

$$\frac{2-\theta}{\theta}\frac{2}{3\sqrt{2\pi}}\rho_s T_{sy} a_{yyy} + \rho_s T_{sy} = \rho_w T_{wy} \quad (11)$$

For the tangential and normal directional energies,

$$\rho_s\sqrt{T_{sy}}T_{sx}\left(1 + \frac{2-\theta}{2\theta}z\sqrt{2\pi}a_{xxy}\right) = \rho_w\sqrt{T_{wy}}T_{wx} \quad (12)$$

$$\rho_s T_{sy}^{3/2}\left(1 + \sqrt{\frac{\pi}{2}}\frac{2-\theta}{2\theta}a_{yyy}\right) = \rho_w T_{wy}^{3/2} \quad (13)$$

The subscript s in the above equations refers to the slip values at the surface, and the subscript w denotes given wall values. The parameter z was found to control the slip value, and was taken $z = \pi$ hereafter. It needs to be mentioned that the expressions for the momentum and energies may be further simplified if single temperature is assumed at the wall, i.e. $T_x = T_y = T_z$. The coefficients in Eqs. (11) and (13) may be determined as

$$a_{xy} = \frac{2}{\nu}A_{xy}R\sqrt{T_x T_y} = -\frac{2}{\nu}R\sqrt{T_x T_y}\left(\frac{1}{RT_y}\frac{\partial u_x}{\partial y} + \frac{1}{RT_x}\frac{\partial u_y}{\partial x}\right),$$

$$a_{xxy} = \frac{2}{\nu} A_{yxx} R^{\frac{3}{2}} \sqrt{T_y}\, T_x = -\frac{1}{6\nu} \frac{\sqrt{RT_y}}{T_x} \left(5\frac{\partial T_x}{\partial x} + 3\frac{\partial T_y}{\partial x} + \frac{\partial T_z}{\partial x} \right),$$

and

$$a_{yyy} = \frac{2}{\nu} A_{yyy} (RT_y)^{\frac{3}{2}} = -\frac{1}{6\nu} \sqrt{\frac{R}{T_y}} \left(\frac{\partial T_x}{\partial x} + 7\frac{\partial T_y}{\partial x} + \frac{\partial T_z}{\partial x} \right).$$

The numerical solution of the equations for the momentum and directional energies provides the required values for the velocity slip and temperature jump at the wall.

SOLUTION OF 1D HEAT TRANSFER PROBLEM FOR LOW TEMPERATURE RATIO

The FiPy finite volume partial differential equation solver [8] is used to integrate Eq. (3). The obtained results are compared with DSMC results computed with SMILE code [9] and a 1D Navier-Stokes (NS) code that incorporates first order temperature slip (jump) at the surface. Consider first the temperature profiles between parallel walls for relatively low hot-wall to cold-wall temperature ratio χ. The results for $\chi = 1.1$ in the slip flow regime are shown in Fig. 1 for two continuum approaches. Hereafter, the Knudsen number, Kn, is defined using the hard sphere interaction model, similar to Ref. [10]. For the 7-moment solutions, not only the total temperature T is shown, but also the temperatures in directions parallel (x) and perpendicular (y) to the wall. As can be expected for such a close to equilibrium flow, the 7-moment and NS solutions are almost identical, with the biggest difference observed at the hot wall. The insert in the left upper corner of Fig. 1 shows the details of the flow in the vicinity of the hot wall. It is seen that the temperature separation, although visible, still does not exceed 0.1% of the corresponding temperature values.

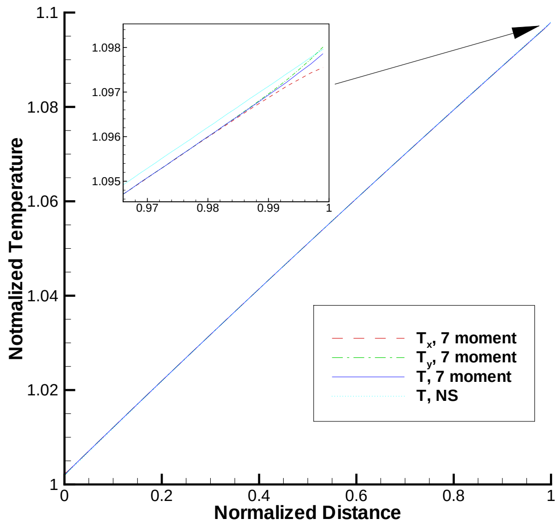

FIGURE 1. Comparison of temperature profiles obtained with NS and 7-moment equations for $\chi = 1.1$ and $Kn = 0.02$.

An increase in temperature ratio and gas density results in a somewhat larger difference between 7-moment and NS solutions, although the solutions are still fairly similar, as shown in Fig. 2 (left). It is interesting to note that the temperature slip values are very close for the continuum solutions, as seen in the insert. Separation of parallel and perpendicular directional temperatures is much more pronounced than for $\chi = 1.1$, and the difference between them reaches 1% at the hot wall. The qualitative behavior of the directional temperatures at the hot wall is qualitatively similar to the DSMC results (Fig. 2, right), with the temperature in the direction parallel to the wall being visibly lower. Note that the slip values of T_x and T_y obtained by the solution of the 7-moment equations are close to those in the DSMC method, although there is some difference in the central region between the plates. Generally, the agreement between 7-moment and DSMC solutions is somewhat better than between NS with slip and DSMC.

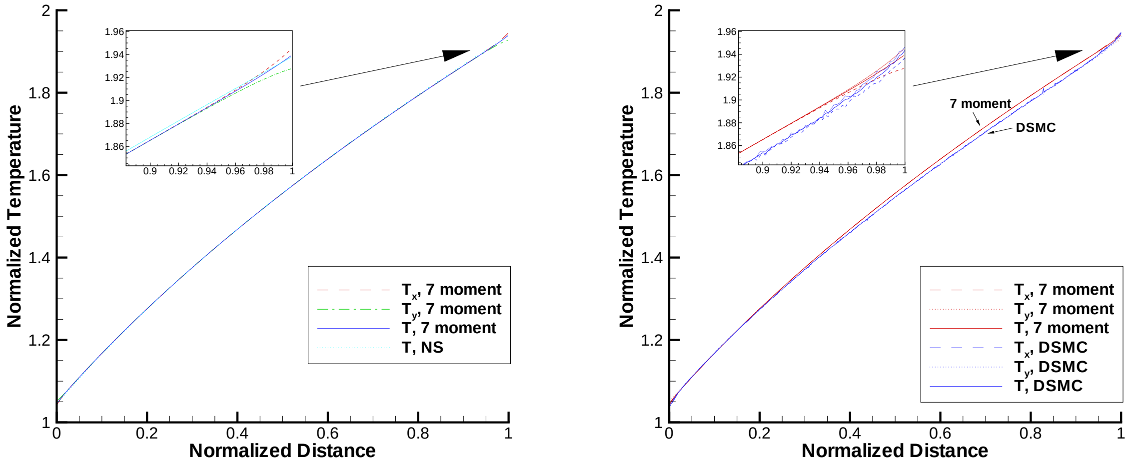

FIGURE 2. Comparison of 7-moment solutions for $\chi = 2$, $Kn = 0.05$ with NS (left) and DSMC (right) results.

SOLUTION OF 1D HEAT TRANSFER PROBLEM FOR HIGH TEMPERATURE RATIO

As may be expected, the difference between the continuum 7-moment solution and the kinetic DSMC method increases with temperature ratio χ due to more significant deviation from equilibrium. Comparison of temperature profiles for different approaches is shown in Fig. 3 (left) for $\chi = 4$. The overall temperature for the 7-moment equation set is close to that obtained by the solution of the NS equations. The directional temperature slip values at both walls are relatively close to the DSMC results, with the longitudinal temperature T_y being lower than T_x at the hot wall and higher than T_x at the cold wall. The thickness of the slip region is also similar in DSMC and 7-moment solutions. However, there is a visible difference in temperatures in the central part of the flow. The components of the heat flux q_{yyy}, q_{yxx} and the total heat flux q_x normalized according to Ref. [10] are shown in Fig. 3 (right). Although the 7-moment equation reproduces the difference between the flux components observed in the DSMC method, and qualitatively correctly predicts the flux profile in the slip layer, it overpredicts the DSMC values by over 10%.

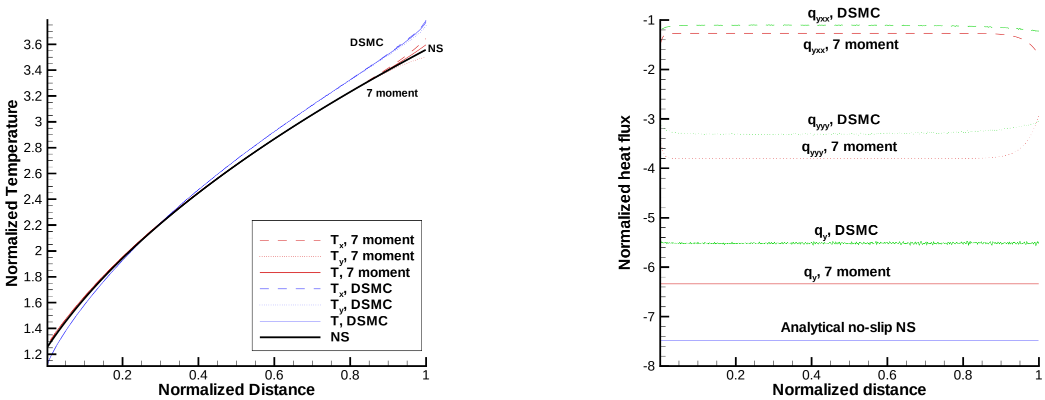

FIGURE 3. Comparison of 7-moment and DSMC temperature profiles (left) and heat fluxes for $\chi = 4$, $Kn = 0.05$.

Comparison between different approaches was also conducted for a rather high temperature ratio of 10. As illustrated in Fig. 4 (left), for a near-continuum flow ($Kn = 0.01$), the directional temperatures at the wall for the 7-moment and DSMC solutions agree very well. Similar to the results presented in the previous section, the larger difference is observed inside the gas volume. Note also that both continuum and kinetic approaches predict the regions where the directional temperatures separate of about 3% of the total separation between plates. The agreement deteriorates as the Knudsen number increases, as illustrated in Fig. 4 (right). In this case, there is also some difference between the 7-moment and DSMC results observed at the cold wall. Similar to the lower temperature ratio cases, the overall temperature for the 7-moment equation set is close to the NS profile.

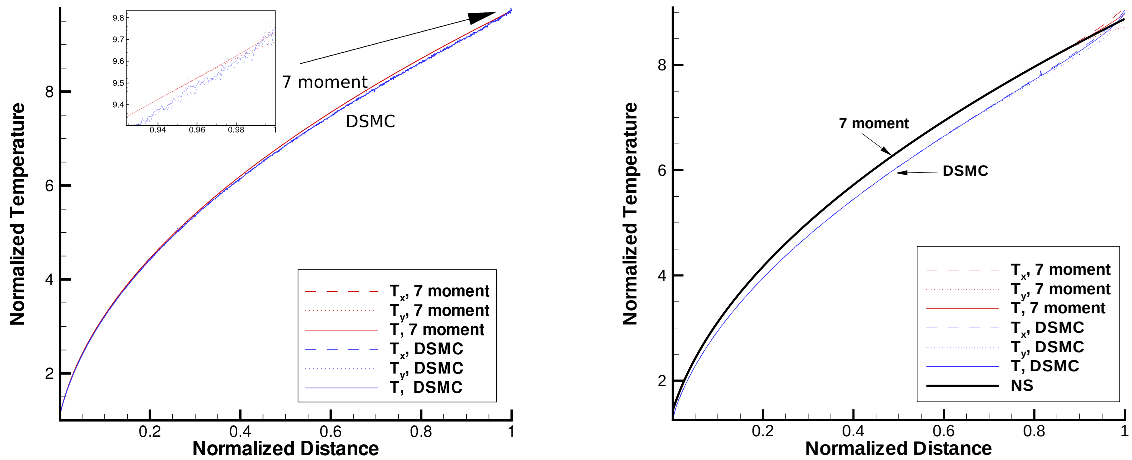

FIGURE 4. Comparison of 7-moment and DSMC temperature profiles for $\chi = 10$, $Kn = 0.01$ (left) and $Kn = 0.05$ right.

CONCLUSIONS

Applicability of gas dynamic equations for 7 moments of the velocity distribution function to predict non-equilibrium flows in slip regime was analyzed for a 1D heat transfer problem. Slip boundary conditions were developed for these equations, and significant directional temperature separation at the cold wall was observed. The obtained results were compared with DSMC predictions, as well as with the solution of NS equations with slip. Good agreement between the 7-moment and DSMC results at the hot wall where the temperature separation is largest, was shown. Significant separation of directional temperatures and heat fluxes at both walls was observed for larger temperature ratios in the 7-moment equation solutions, and results qualitatively agree with the DSMC predictions.

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