Analysis of Rotational Nonequilibrium in Standing Shock Waves of Nitrogen

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Introduction

THERMAL nonequilibrium occurs when the temperatures associated with the translational, rotational, and vibrational modes of a polyatomic gas are unequal. Recently, it has been shown by Boyd[1] that such phenomenon plays a significant role in determining the macroscopic flow quantities that exist in front of a hypersonic space vehicle under rarefied conditions. The one-dimensional standing shock wave represents the simplest flow in which nonequilibrium effects may be considered, and it is for this reason that such flows have been examined both theoretically and experimentally for a number of years. Experimental measurements of shock waves for diatomic nitrogen were made by Robben and Talbot.[2] In these experiments, density, rotational temperature, and rotational energy distributions were obtained. The flow conditions gave a stagnation temperature of 300 K, which ensured that the vibrational and chemical states of the gas could be assumed to be frozen. Previous attempts to model this data using continuum methods and kinetic theory[3,4] met with limited success. These approaches were unable to provide general solutions for all conditions and required suitable selection of the rotational relaxation number Z_R. Bird (see Ref. 5, p. 189) produced a solution for a weak shock wave, with a Mach number of 1.7 in nitrogen, by using the direct simulation Monte Carlo method (DSMC) and obtained excellent agreement with results reported in Ref. 2 for both density and rotational temperature. These results were calculated using an energy sink model in which the transfer of energy between the translational and rotational modes is performed in such a way as to push these energy modes toward equilibrium. In the weak shock, it is clear that this technique is sufficient; however, it is doubtful that it would be as successful in stronger shocks that exhibit a more significant degree of thermal nonequilibrium.

In the current work, the DSMC technique is also employed, and energy is transferred between the translational and rotational modes by using the Borgnakke-Larsen phenomenological model.[6] This method assumes that a fraction ϕ of all collisions are inelastic and, therefore, involve energy transfer. The postcollision values are determined by sampling from the appropriate equilibrium distribution functions, as described in Ref. 6. Previously, in the majority of DSMC calculations involving rotational nonequilibrium, it has been assumed that ϕ is a constant for all of the computational domain and has been defined as the reciprocal of the rotational collision number. Temperature-dependent expressions for the energy exchange probability have been introduced by Davis et al.[7] and more recently by Boyd.[8] It is the purpose of this Note to further develop the model described in Ref. 8 and to make calculations that can be compared directly with experimental data.

Variable Exchange Probability Model

The following continuum expression for the rotational collision number was derived by Parker[9]:

$$Z_R = \frac{(Z_R)_\infty}{1 + (\pi^{3/2}/2)\,(T^*/T)^{1/2} + [(\pi^2/4) + \pi]\,(T^*/T)} \tag{1}$$

where T^* is the characteristic temperature of the intermolecular potential and $(Z_R)_\infty$ is the limiting value. Although Parker's expression is derived from an analysis involving a large number of assumptions, the temperature-dependent nature of Eq. (1) is in agreement with the more rigorous treatment of Lordi and Mates[10] who performed classical trajectory calculations. The values of $(Z_R)_\infty$ and T^* are chosen so as to obtain the best correspondence between Parker's expression and the results of Ref. 10. Belikov et al.[11] have shown that the model best represents the experimental data for a range of temperature. It has been shown by Boyd[8] that Eq. (1) may be reproduced in a discrete particle simulation by assuming that the probability of energy exchange is a function of the relative velocity of collision c_r. An expression for the instantaneous exchange probability must then be found that reduces to Eq. (1) when integrated over the equilibrium distribution function for the translational collision energy for all possible collisions. The expression for the energy exchange probability is given in Ref. 8 as

$$\phi_R \frac{(Z_R)_\infty}{Z_t} = 1 + \frac{\Gamma(2-\omega)}{\Gamma[(3/2)-\omega]} \left(\frac{2kT^*}{m_r c_r^2}\right)^{1/2} \frac{\pi^{3/2}}{2}$$

$$+ \frac{\Gamma(2-\omega)}{\Gamma(1-\omega)} \left(\frac{2kT^*}{m_r c_r^2}\right) \left(\frac{\pi^2}{4} + \pi\right) \tag{2}$$

where m_r is the reduced mass of the collision, k the Boltzmann constant, Z_t the translational collision number, and ω the parameter in the variable hard sphere model of Bird,[12] which determines the nature of the interaction potential.

In their analysis, Lordi and Mates[10] found that nonequilibrium between the translational and rotational modes affects the rotational collision number. Specifically, when the rotational temperature exceeds that for the translational mode, which occurs in freejet expansions, the exchange probability is reduced in comparison to that obtained when the two modes are in equilibrium. Clearly, the opposite will be true for compression flow where the translational temperature leads the rotational temperature. Therefore, to account for such effects, it is necessary to determine the exchange probability as a function of both the rotational and translational energies that occur at each collision. This is achieved by employing the equilibrium distribution function for the total collision energy[13]:

$$f\left(\frac{E_c}{kT}\right) = \frac{1}{\Gamma(\zeta + 2 - \omega)} \left(\frac{E_c}{kT}\right)^{\zeta + 1 - \omega} \exp\left(-\frac{E_c}{kT}\right) \tag{3}$$

In Eq. (3), E_c is the sum of the translational and internal collision energies and ζ is the average number of degrees of freedom of the colliding molecules. Using this function, it may be shown that Parker's result is reproduced under equilibrium

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conditions with the following instantaneous exchange probability:

$$\phi_R \frac{(Z_R)_\infty}{Z_t} = 1 + \frac{\Gamma(\zeta+2-\omega)}{\Gamma[\zeta+(3/2)-\omega]}\left(\frac{kT^*}{E_c}\right)^{1/2}\frac{\pi^{3/2}}{2}$$

$$+\frac{\Gamma(\zeta+2-\omega)}{\Gamma(\zeta+1-\omega)}\left(\frac{kT^*}{E_c}\right)\left(\frac{\pi^2}{4}+\pi\right) \tag{4}$$

To consider the behavior of this model under nonequilibrium conditions it is useful to regard the temperature T in Eq. (1) as the weighted average of the translational and rotational temperatures. In the case where the translational temperature is greater than the rotational value, then the weighted temperature will be less than the translational value. Evaluation of Eq. (1) with these temperatures will then show that the collision number obtained with the weighted temperature is less than that obtained with the translational temperature. Alternatively, it may be stated that the collision probability obtained with the weighted temperature is greater than the translational temperature result.

Parker's expression in Eq. (1) gives a similar temperature dependence to that proposed by Davis et al.[7] for nitrogen. The form of the exchange probability given in Ref. 7 was obtained by a best-fit to the available data. However, the model proposed in the current work represents an improvement in that the exchange probability is defined explicitly in terms of molecular quantities, so that it may be applied to any gas. In addition, the model employed in Ref. 7 does not reach equipartition.

Results

The first calculation considered matches the experimental conditions for the Mach 1.71 shock wave investigated by Robben and Talbot.[2] In Fig. 1, the structure of the rotational temperature through the shock is shown. The distance through the shock is normalized to the upstream mean free path. For the case in which the exchange probability is kept constant ($Z_r = 5$), it is clear that the rotational temperatures are slightly underestimated in the downstream portion of the shock. The introduction of Eq. (4) into the calculations is found to give excellent correspondence to the experimental data. Although the differences in the calculated results are small, it should be noted that the simulation of this weak shock wave, where the degree of thermal nonequilibrium is small, represents a much simpler problem than the flow conditions experienced by reentering spacecraft. Therefore, it is found that the constant probability model is incapable of correctly predicting rotational nonequilibrium in the most elementary flows. The exchange probability calculated with Eq. (4) through the shock was found to vary between 0.33 at the upstream boundary to about 0.27 in the downstream section. The fact that the exchange probability is always greater than 0.2 implies that a greater amount of energy will be transferred from the translational to the rotational mode. In this way, the rotational temperature profile calculated with Eq. (4) is lifted above that obtained with the constant probability model to the level observed in the experiment.

The new model has also been tested in a Mach 7 shock wave in which significant nonequilibrium exists. Once again, the flow conditions were chosen to match those investigated experimentally in Ref. 2. Results were generated with a constant probability, with Eqs. (2) and (4), and these are shown in Fig. 2. An improvement in the correspondence between the experiment and the calculations is clearly seen with the introduction of Eq. (2). A further significant improvement is subsequently obtained with Eq. (4), thereby indicating the usefulness of the new formulation. Once again, the constant probability model predicts rotational temperatures that are lower than those observed experimentally. It should also be noted that when the

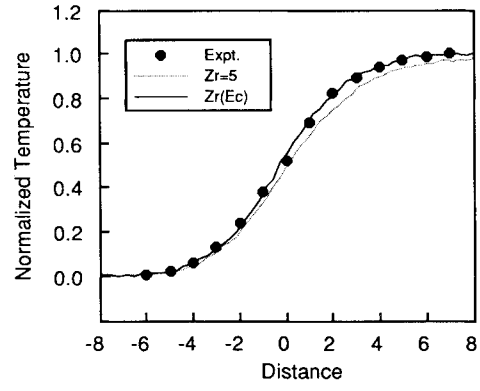

Fig. 1 Normalized rotational temperatures in a Mach 1.71 shock wave in nitrogen.

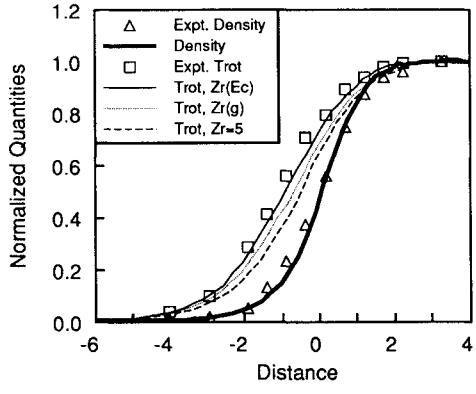

Fig. 2 Normalized flow quantitites in a Mach 7 shock wave in nitrogen.

rotational temperature lags behind the translational temperature, the effect of employing Eq. (4) is to decrease the rotational collision number. This feature of the model is in quantitative agreement with the findings of Ref. 10, as discussed earlier.

Conclusions

Theoretical predictions of rotational temperature calculated using a new variable energy transfer probability model in the DSMC technique are found to give excellent agreement with experimentally obtained profiles in shock waves of nitrogen. The previous approach of employing a constant exchange probability is found to give a much poorer correspondence. It is therefore concluded that the use of the model described in this paper is preferred in flows where rotational nonequilibrium plays a significant role.

Acknowledgment

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New Mixing-Length Model for Supersonic Shear Layers

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Introduction

EARLY experiments on supersonic free shear layers revealed the inverse relationship between spreading rate and increasing Mach number.[1] It was thought that the reduction in spreading rate at high Mach number was due to a density effect. The experiments by Brown and Roshko[2] had shown that there is some effect of density ratio on spreading rate; however, the effect is much smaller than that observed in supersonic shear layers.

In an attempt to correlate the various data on high-speed shear layers, Bogdanoff[3] introduced the concept of the convective Mach number, which in effect casts the data into a frame convecting at the velocity of the large eddies of the mixing layer. Many investigators had attempted to incorporate compressibility effects in turbulence models, but their attempts were essentially a curve fit of spreading rate vs Mach number data, and a subsequent damping of the eddy viscosity.

A new mixing-length model has been developed without empirically fitting the data. A rationale is presented for prescribing the mixing length which reduces to the well-established incompressible form for subsonic flows, and produces the correct spreading behavior as the Mach number is increased above unity.

Theory

From Prandtl's mixing-length theory, the turbulent viscosity can be written as follows[4]:

$$\mu_t = \rho \ell^2 \left|\frac{\partial u}{\partial y}\right| = \rho C^2 L^2 \left|\frac{\partial u}{\partial y}\right| \tag{1}$$

where ℓ is the mixing length. The mixing length is generally the product of an empirically determined constant C and some characteristic scale L of the mixing region. For incompressible shear-layer calculations, the shear-layer width δ serves as the characteristic length and the value of the constant ranges from 0.05 to 0.09. When the above formula is used for calculation of free shear layers at high Mach number, it fails to predict the reduced spreading rate. It is thus felt that compressibility effects should be included in the mixing-length definition. The main difference between incompressible and supersonic shear layers is that, at some regions in supersonic shear layers, relative supersonic flow can exist. A relative supersonic flow exists at a given axial location when there is a flow which moves supersonic relative to the other flows within the shear layer. The mixing length for a turbulent shear layer can be interpreted analogous to the mean free path of a molecule in the derivation of the laminar viscosity from kinetic theory. The mixing length can then be assumed proportional to some distance over which a disturbance can propagate or penetrate.

In subsonic shear layers there is no relative supersonic flow, therefore the characteristic scale L can be assumed to be δ. For supersonic shear layers, L can be assumed to be the distance between the points where flow moves sonic relative to the local point, at a given streamwise station. Figure 1 shows a velocity profile for a supersonic shear layer, At a given point y, where the velocity is u and the speed of sound is a, one can find the locations, Y_a and Y_b, where the flow is moving sonic relative to the point y with a limitation that Y_a and Y_b cannot exceed the edges of the shear layer, Y_{el} and Y_{eu}. If a relative sonic flow exists, the values of $|(u_a - u)/a|$ and $|(u_b - u)/a|$ are unity and L is $|Y_a(y) - Y_b(y)|$. Using the above assumption, the turbulent viscosity for supersonic shear layers can be written as follows:

$$\mu_t = \rho C^2 C_s^2 L^2(y) \left|\frac{\partial u}{\partial y}\right| \tag{2}$$

where $L(y)$ is the new characteristic scale obtained as described and C_s is a constant which can be determined from experimental data. By matching the calculated spreading rate parameter for a Mach 5 free shear layer to 37, which was obtained experimentally, the value of 0.89 was obtained for C_s. If there is no relative supersonic flow within the shear layer, C_s becomes unity.

Results and Discussion

To verify the new mixing-length model, a two-stream air mixing layer with the following conditions was calculated:

p is constant across shear layer and $T_{t1} = T_{t2}$
$P_r = 0.72$, $P_{rt} = 0.9$, and $T_1 = 300°$ K
$M_1 = 0.1$, 1, 2, 3, 4, 5 and $Re\,1/m = 2.2 \times 10^7$
$u_2/u_1 = 0.005$, $C = 0.085$ and $C_s = 0.89$

The boundary-layer code STAN5[5] with the following two definitions of L were used for the calculations:

$$L_a = Y_{0.99} - Y_{0.01} \tag{3}$$

$$L_b = L(y) \text{ from Fig. 1} \tag{4}$$

Y_s is the y coordinate where $(u - u_2)/(u_1 - u_2) = s$ and Y_{eu} and Y_{el} are the edges of the shear layer, $Y_{0.99}$ and $Y_{0.01}$, respectively.

L_a is from the incompressible mixing-length model in Eq. (1) and L_b is from the new mixing-length model in Eq. (2). To calculate the spreading-rate parameter, the following formula was used:

$$\sigma = F \times 1.855 \times (X_a - X_b)/(DY_a - DY_b) \tag{5}$$

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