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Summary

The influence of thermal nonequilibrium in rarefied hypersonic flows has been considered. In a compressed flow, such as a shock wave, typical relaxation effects cause the rotational and vibrational temperatures of molecules to lag behind that for the translational energy mode. In the energetic flowfields which surround reentering spacecraft thermal nonequilibrium effects are most important due to their influence on the chemical activity of the gas. The application of Computational Fluid Dynamics techniques to such flowfields must be treated with great care. At altitudes greater than about 80km above the Earth's surface the rarefied nature of the ambient atmosphere makes the use of traditional continuum techniques inappropriate and resort must be made to particle simulation methods. The manner in which energy exchange between the various energy modes is modelled in the particle simulation is clearly of great importance. A new model for calculating the probability of energy exchange between the translational and rotational modes has been developed. A full description of this work is contained in Appendix A which has been submitted for publication in The Physics of Fluids. The role of vibrational energy exchange has also been investigated. A model for determining the probability of energy transfer to the vibrational modes has also been derived. This model, together with that described in Appendix A, have been incorporated into a one-dimensional study of the flow of air past a blunt body at an altitude of 90km. The results of this study are discussed in

Appendix B. This material was presented at the 20th AIAA Fluid Dynamics, Plasma Dynamics, and Lasers Conference, Buffalo, NY, June 1989, and has been submitted for publication to The Journal of Thermophysics and Heat Transfer.

APPENDIX A

ROTATIONAL-TRANSLATIONAL ENERGY TRANSFER IN RAREFIED NONEQUILIBRIUM FLOWS

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Abstract

A new model for simulating the transfer of energy between the translational and rotational modes ~~is~~ was derived for a homogeneous gas of diatomic molecules. The model ~~has been~~ was developed specifically for use in discrete particle simulation methods where molecular motion and intermolecular collisions are treated at the molecular level. In such methods it is normal to assume a constant rotational collision number for the entire flowfield. The new model differs in that a temperature dependence is introduced which has been predicted by theory and observed in experiment. The new model is applied to the relaxation of rotational temperature, and is found to produce significant differences in comparison with the model normally employed at both high and low temperatures. Calculations have also been performed for a Mach 7 normal shock wave. Large differences in the solutions are again observed, with the new model offering an improved correspondence to the available experimental data.

PACS Numbers

34.50.Ez Rotational Energy Transfer.
47.45.-n Rarefied Gas Dynamics.
02.70.+d Computational techniques.
47.40.Nm Shock waves.

I. Introduction

The use of discrete particle simulation methods in fluid mechanics has become widespread with the recent increase in interest in rarefied, nonequilibrium gas flows. This interest has mainly been concerned with high altitude rocket and thruster expansion plumes[1,2], and with the flowfield surrounding a space vehicle as it re-enters the Earth's atmosphere at high velocity[3]. The most commonly applied particle simulation technique is that developed by Bird[4] and is termed the Direct Simulation Monte Carlo method (DSMC). This solution scheme proceeds by modelling all physical and chemical phenomena at the molecular level, and is therefore preferred to more traditional continuum formulations when rarefied effects become important.

One of the most significant effects observed in rarefied flowfields is the presence of a large degree of nonequilibrium between the various internal energy modes of the gas. It is therefore of great importance that such phenomena are adequately simulated within the DSMC technique. Presently, the exchange of energy between translational, rotational, and vibrational modes in the DSMC method is treated in a simplistic manner which relies more on convenience than any physical basis. In particular, the existing models fail to allow the collision numbers associated with the rotational and vibrational modes to exhibit any temperature dependence.

The purpose of the present work is to improve the modelling of translational-rotational energy exchange for use in discrete particle simulation methods. A temperature dependent collision number employed in continuum calculations is used as a basis to develop a model which reproduces equilibrium behaviour in results obtained with the DSMC technique. The new model is then applied to a simple relaxation problem, and to a strong shock wave in which a significant temperature range exists.

II. Translational-Rotational Energy Exchange

In a gas of colliding molecules, energy is continually being transferred between the various internal modes. These collisions tend to push the internal energy distributions towards their equilibrium state. The number of collisions required to equilibriate a particular mode of each molecule is called the collision number Z of that mode. Each internal mode has a separate collision number, and it is generally the case that

$$Z_{translation} < Z_{rotation} < Z_{vibration}$$

It therefore takes a greater number of collisions for the rotational mode to reach equilibrium than the number required for translational energy. Thus, if the collision rate in any reference volume in the flowfield does not allow each molecule to collide $Z_{rotation}$ times before leaving, then nonequilibrium exists in that volume. In the treatment of rotational energy exchange between the translational and rotational modes, the following expression is often employed in continuum calculations:

$$\frac{dE_R}{dt} = \frac{E_R^* - E_R}{\tau_R} \tag{1}$$

where E_R is the rotational energy, E_R^* is the equilibrium value, and τ_R is the rotational relaxation time which is generally regarded as being a function of temperature and pressure (or density).

While Eq.(1) is suitable for continuum calculations, it is inappropriate for use in particle simulation schemes in which all macroscopic flow properties are derived by averaging molecular properties over large sample sizes. The particle simulation technique considered here is the Direct Simulation Monte Carlo method. In this technique, the large number of molecules in a real gas are simulated by a much smaller representative set of model particles. The motion of these particles is followed through physical space and intermolecular collisions are treated on a probabilistic basis. Several different collision schemes have been developed and most of these have been categorised by Nanbu^5. The scheme employed in the present work is the Time Counter method of Bird which has the combined advantages of numerical efficiency and low statistical fluctuations (see Ref. 6).

In addition to retaining molecular velocities, it is possible to simulate the internal energy modes associated with polyatomic gases. In order to avoid the complexities of computing individual transitions between the various internal quantum states, a continuous distribution of internal energies is usually assumed. While the rotational energy of a molecule should be simulated by considering its angular velocity vector, it is computationally simpler to ignore all effects due to the orientation of the colliding bodies. Thus, it is usual to associate a scalar rotational energy value with each molecule.

Rotational energy exchange schemes involving classical laws of mechanics have been proposed by MacPherson[7] and individual quantum level transition probabilities for nitrogen have been calculated by Deiwert and Yoshikawa[8]. Both of these methods suffer from computational overheads which prohibit their use in discrete particle simulations of complex flowfields.

In a particle simulation scheme it is more economical to employ the concept of a collision number in preference to either Eq.(1) or the work described in Refs. 7 and 8. The rotational collision number is usually defined as

$$Z_R = \frac{\tau_R}{\tau_c} \tag{2}$$

where τ_c is the mean time between collisions. The transfer of energy between the various modes is usually implemented into the DSMC technique using the Larsen-Borgnakke phenomenological model[9]. In this model, a fraction ϕ of all collisions are considered to be inelastic and the remaining (1 - ϕ) collisions are treated as perfectly elastic spheres. If the collision number Z of an internal mode is given by Eq.(2), then the probability of energy exchange involving this mode, ϕ, is conveniently defined as

$$\phi = \frac{Z_t}{Z} \tag{3}$$

where Z_t is the translational collision number. It is usual in DSMC calculations to take Z_t to be equal to unity and Z_R=5, so that a constant value of ϕ_R=0.2 is obtained. This value for Z_R has been chosen to coincide with results obtained from ultrasonic[10] and shock wave[11] experiments. The calculation of an inelastic collision is then performed by statistically sampling values using the equilibrium distribution functions together with the total collision energy (including internal mode contributions).

By assuming that the rotational collision number is constant over the entire flowfield, any temperature dependence is thereby neglected. This concept is in direct opposition to the theoretical findings of Parker[12], and Lordi and Mates[13], and the experimental data of Carnevale et al[14]. Parker has used an empirical non-impulsive potential model which incorporates a small degree of asymmetry to derive an expression for the rotational relaxation time τ_R. By initially assuming that there is zero energy in the rotational modes of a gas of homonuclear diatomic molecules, the following approximate expression is obtained:

$$Z_R = \frac{(Z_R)_\infty}{1 + \frac{\pi^{\frac{3}{2}}}{2}\left(\frac{T^*}{T}\right)^{\frac{1}{2}} + \left(\frac{\pi^2}{4} + \pi\right)\frac{T^*}{T}} \tag{4}$$

where T* is the characteristic temperature of the intermolecular potential, and $(Z_R)_\infty$ is the limiting value.

While Parker's expression is derived from an analysis involving a large number of assumptions, the temperature dependent nature of Eq.(4) is in agreement with the more rigorous treatment of Lordi and Mates who performed classical trajectory calculations. In the current work the value of $(Z_R)_\infty$ is chosen so as to obtain the best correspondence between Parker's results and those of Lordi and Mates.

A previous attempt to introduce a temperature dependent nature of the rotational collision number into DSMC calculations was reported by Davis et al[15]. It was proposed that Z_R should be specified as a function of the total collision energy of the colliding molecules, i.e. the sum of translational and rotational collision energies. The exact derivation of the expression employed is omitted and the model fails to satisfy the principle of detailed balance. It is therefore the intention here to derive an expression from Eq.(4) which may be utilized in discrete particle simulations.

III. Probability of Translational-Rotational Energy Exchange

In the following, the principal aim is to derive an expression for the reciprocal of the rotational collision number from the molecular collision properties of the gas. A decision must therefore be made on the collision parameter best suited for this purpose. As Eq.(4) is strictly a function of translational temperature this suggests that the relative velocity of collision, c_r, should be employed. For an equilibrium gas, it may be shown that the average value of a quantity Q which is a function of c_r alone may be expressed as

$$< Q >= \frac{2\left(\frac{m_r}{2kT}\right)^{2-\omega}}{\Gamma(2-\omega)} \int_0^\infty Q {c_r}^{3-2\omega} exp\left(\frac{-m_r {c_r}^2}{2kT}\right) dc_r \qquad (5)$$

where m_r is the reduced mass of the collision and ω is a constant used in the Variable Hard Sphere (VHS) collision model of Bird[16] and is related to the viscosity temperature exponent ζ by $\omega = \zeta - 0.5$. In the VHS model the collision mechanics are treated in the same manner as for hard spheres while the total collision cross section is a function of the relative velocity and is given as

$$\sigma_T = \sigma_o\left(\frac{\frac{1}{2} m_r {c_r}^2}{(2-\omega) kT_o}\right) \qquad (6)$$

where σ_o is a reference collision cross section defined at temperature T_o. In this formulation, a value of $\omega = 0$ corresponds to the hard sphere intermolecular potential and $\omega = 0.5$ gives the Maxwell molecule.

The probability that a molecule transfers energy between its translational and rotational modes due to a collision is given by the reciprocal of Eq.(4) which may be written as

$$\phi_R = a_1 + \frac{a_2}{T^{\frac{1}{2}}} + \frac{a_3}{T} \qquad (7)$$

where a_1, a_2, a_3 are constants. To reproduce the global expression of Eq.(7) in a discrete particle simulation, an appropriate form of Q must be found for the integration shown in Eq.(5). Let us assume that each of the three terms on the right hand side of Eq.(7) may be obtained in this way be choosing a general condition $Q=bc_r{}^n$. Thus

$$<Q>=\frac{2b\left(\frac{m_r}{2kT}\right)^{2-\omega}}{\Gamma(2-\omega)}\int_0^\infty c_r{}^{n+3-2\omega}\, exp\left(\frac{-m_r c_r{}^2}{2kT}\right)dc_r \qquad (8)$$

By making the substitution $x=\frac{m_r c_r{}^2}{2kT}$, Eq.(8) becomes

$$\begin{aligned}<Q> &= \frac{b\left(\frac{2kT}{m_r}\right)^{\frac{n}{2}}}{\Gamma(2-\omega)}\int_0^\infty x^{\frac{n}{2}+1-\omega}\, exp(-x)\,dx \\ &= \frac{b\Gamma(2-\omega+\frac{n}{2})}{\Gamma(2-\omega)}\left(\frac{2kT}{m_r}\right)^{\frac{n}{2}} \qquad (9)\end{aligned}$$

On examination of Eq.(9) it becomes clear that the values of n which must be employed for each of the terms in Eq.(7) are 0, -1 and -2 respectively. Therefore, the full expression for the average value of probability for energy exchange between the translational and rotational modes is

$$\begin{aligned}\phi_R\frac{(Z_R)_\infty}{Z_t} &= 1+\frac{\Gamma(2-\omega)}{\Gamma(\frac{3}{2}-\omega)}\left(\frac{2kT^*}{m_r c_r{}^2}\right)^{\frac{1}{2}}\frac{\pi^{\frac{3}{2}}}{2} \\ &\quad +\frac{\Gamma(2-\omega)}{\Gamma(1-\omega)}\left(\frac{2kT^*}{m_r c_r{}^2}\right)\left(\frac{\pi^2}{4}+\pi\right) \qquad (10)\end{aligned}$$

The form of Eq.(10) shows that there is a singularity at $c_r=0$. However, the collision probability for a pair of molecules which have zero relative velocity is itself zero, so that this case does not present a problem. The application of this equation in a DSMC calculation to a number of test cases is considered in the following Sections.

IV. Calculations

To assess the validity, and the significance, of the energy exchange model proposed in the previous Section, the expression in Eq.(10) has been implemented into a number of DSMC calculations. In the present study, a value of $Z_t = 1.5$ has been employed in accordance with the result of Fritzsche and Cukrowski[17]. The first problem undertaken involves a heat bath of nitrogen molecules which are initially in thermal equilibrium. The values employed in Eq.(4) for nitrogen which best correspond to the calculations of Lordi and Mates are T^*=91.5K and $(Z_R)_\infty$=23.5. To begin with, Eq.(10) was employed in such a way that the relative velocity of a given collision determined the instantaneous probability of energy transfer. However, such a procedure fails to preserve the equipartition of the translational and rotational modes. This is because energy exchange then occurs for collisions which have a lower than average translational energy. It was therefore necessary to employ a value for ϕ_R which is averaged over every collision regardless of whether energy exchange actually occurs. This procedure has been tested over a range of temperatures and some example calculations for the values of Z_R derived from the DSMC results together with Eqs.(3) and (10) are shown in Fig. 1. It is clearly shown that the results obtained at the molecular level are found to match Eq.(4) almost exactly.

Having established the fact that Eq.(10) reproduces the continuum result under equilibrium conditions, it is relevant to consider the application of the model to some nonequilibrium problems. The first of these models translational and rotational temperature relaxation in a homogeneous gas. Initially, the rotational energy is set to zero, and the translational temperature is given by 5/3 of the final equilibrium value. As time marches forward in the simulation, the temperatures in the translational and rotational modes will converge to the equilibrium result. This relaxation problem is therefore unsteady, so that the reduction of statistical fluctuations is achieved by averaging results over many complete runs from start to finish.

Relaxation profiles obtained with ϕ_R=0.2 and Eq.(10) are shown in Fig. 2 for rotational temperature. The working gas is nitrogen, and time is normalized with respect to the mean time between collisions at the equilibrium temperature which is 300K in this case. It is seen that small distinguishable differences occur in the results calculated by the two energy transfer models. For the translational temperature range considered in this calculation, the value for ϕ_R obtained from Eq.(10) is greater than 0.2. The rate of transfer of energy to the rotational modes is therefore greater, and the rotational temperature converges to the equilibrium value in a shorter time. Another important feature of the results shown in Fig. 2 is that equipartition of the thermal modes is achieved at equilibrium with the new model. In Fig. 3 the rotational relaxation history is shown, this time for a final temperature of 5000K. Under these conditions, the values of ϕ_R calculated with Eq.(10) are much less than 0.2, and so the relaxation process is slower.

Unfortunately, the results shown in Figs. 2 and 3 cannot be verified experimentally. However, these theoretical calculations indicate that significant differences occur due to the introduction of a temperature dependent collision number. It is therefore appropriate to make calculations of a flow for which rotational temperature measurements are available. Assessment has been made of the differences found for the solutions obtained with the two models in the calculation of a strong shock wave. The two different sets of conditions investigated are listed in Table I and the working gas is again nitrogen. The first set of conditions has been chosen to match the experimental data of Robben and Talbot[11] who produced a number of shock waves in a wind tunnel by expanding a jet through a shock-holder. The high Mach number shock waves studied by Robben and Talbot are much thinner than those produced by Alsmeyer[18] in a shock-tube. The explanation for this phenomenon lies in differences in the upstream flow conditions in the two experiments. In Alsmeyer's study, the upstream conditions should ensure the existence of thermal equilibrium. To obtain high Mach number shock waves, it was necessary for Robben and Talbot to allow the expanding jet to undergo significant rarefaction. In such expansions the translational temperature will normally relax more efficiently than the rotational mode (see Ref. 2). Thus, at the upstream boundary, the translational temperature will probably be less than the value of 28K obtained for the rotational temperature.

In the present calculations, thermal equilibrium is assumed at the upstream boundary. To reproduce the thin shock wave of Robben and Talbot it is necessary to employ an unusually low viscosity temperature exponent. Such an undertaking leads to a reduction in the molecular collision rate which is quantitatively consistent with the upstream translational temperature being lower than that for rotation.

The simulation procedure employed follows that of Bird[19]. The profiles for density and temperature are shown in Fig. 4, and have been normalized as follows:

$$\overline{\rho} = \frac{\rho - \rho_1}{\rho_2 - \rho_1} \qquad (11)$$

$$\overline{T} = \frac{T - T_1}{T_2 - T_1} \qquad (12)$$

The calculated density profiles obtained with each of the energy transfer models were found to be exactly consistent. Therefore, only the result obtained with Eq.(10) is shown, and it is evident that excellent agreement is found with the experimental data. The reciprocal shock wave thickness for the density profile is about 0.41 which is in good agreement with the value derived by Alsmeyer[18] for the data of Robben and Talbot. The correspondence between the theoretical and experimental results for rotational temperature is not as good. Significantly, the profile obtained with the new model shows an improvement of up to 20% on that calculated with ϕ_R=0.2. The results shown in Fig. 4 indicate that the new energy transfer may be successfully applied in a discrete particle simulation, and gives better correspondence to experimental data.

A further set of calculations has been made for a Mach 7 shock wave where the upstream temperature is taken to be 300K and less rarefied conditions are assumed. This allows assessment of the effect of the new energy transfer model when the collision number is greater than 5 and gives conditions similar to those investigated by Alsmeyer[18] using a shock tube. The assumption of thermal equilibrium in the upstream portion of the flowfield is now more certain. The normalized density profiles obtained by implementing Eq.(10) for the two sets of conditions are shown in Fig. 5. The effect of simulating a shock tube study is to increase the shock layer thickness and occurs because of differences in the rate of rotational energy exchange and viscosity effects. The calculated value for the reciprocal shock thickness again shows good agreement with that which may be deduced from Ref. 18.

The normalized profiles for translational and rotational temperature obtained from these simulations are shown in Fig. 6. For the range of temperature found in this simulation it is observed that more significant differences exist for the two solutions. As expected, the rate of transfer of energy to the rotational modes is reduced by application of Eq.(10). It should be noted that the differences between the results obtained with the two energy transfer models will increase as the translational energy in the flowfield is increased. It is therefore proposed that the new model may have significant impact on re-entry calculations such as those presented in Ref. 3 where the translational temperature may exceed 30,000K.

Concluding Remarks

The introduction of a temperature dependent collision number into discrete particle simulation schemes has been found to be significant. Even for the simple case of relaxation in a homogeneous gas differences are discernible between the results obtained with the new model and those calculated under the assumption that the collision number is everywhere equal to 5. The application of the new model to a shock wave problem under very rarefied conditions gives improved correspondence with experimental data in comparison to a constant collision number. It is concluded that the new model should be preferred in calculations which involve a significant degree of rotational nonequilibrium. Finally, it should be noted that the model presented here may also be used to allow separate rates of translational-rotational energy exchange between the different molecules in a gas mixture.

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Table I. Upstream conditions for Mach 7 shock wave calculations.

ρ_1 (kg m^{-3})	T_1 (K)	u_1 (ms^{-1})
$3.12\mathrm{x}10^{-5}$	29	764
$7.77\mathrm{x}10^{-3}$	300	2470

Figure Legends

Fig. 1 Rotational collision number obtained from Eq.(3) and Eq.(10).

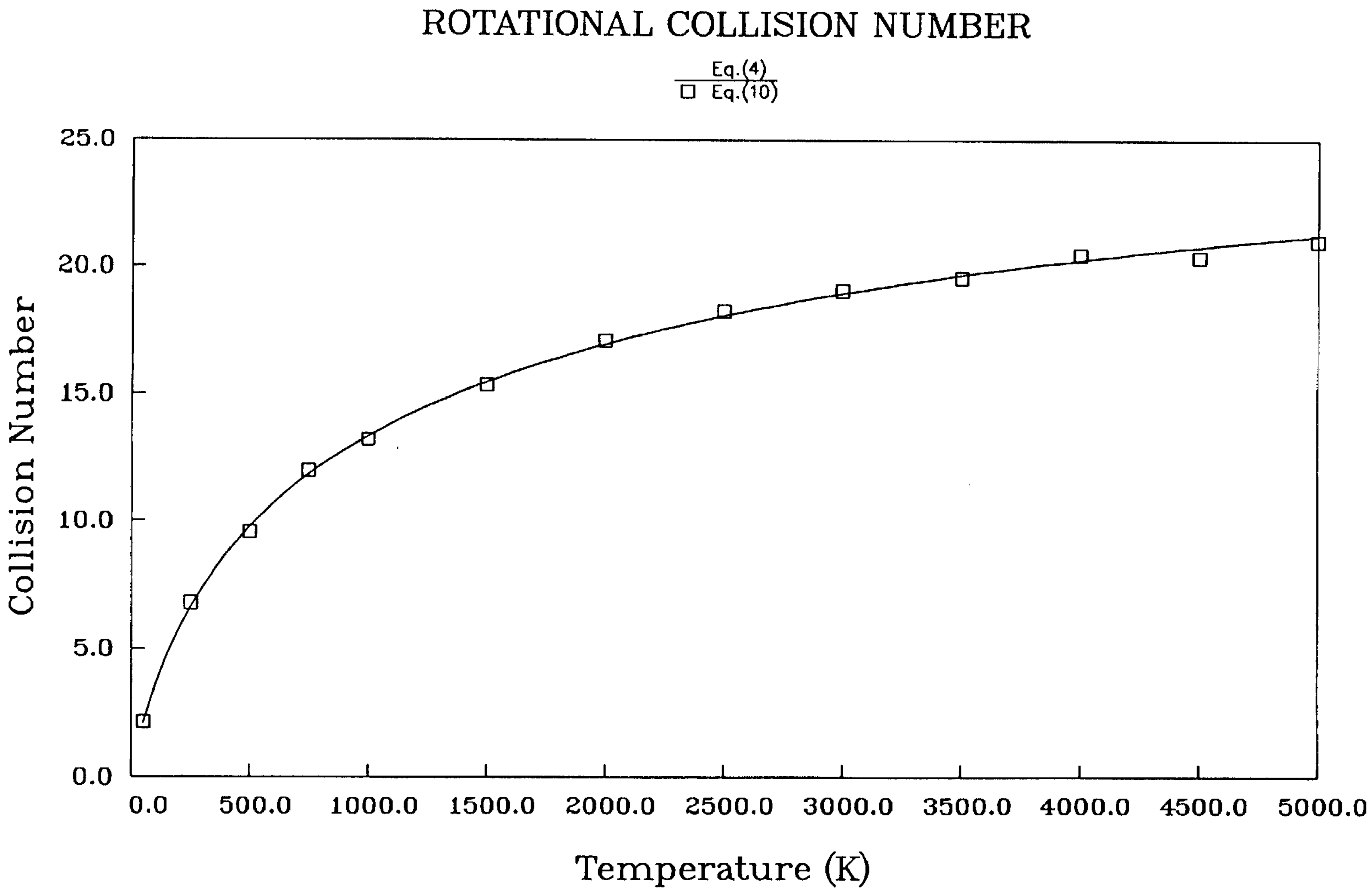
Fig. 2 Homogeneous relaxation of the rotational temperature of nitrogen at 300K.

Fig. 3 Homogeneous relaxation of the rotational temperature of nitrogen at 5000K.

Fig. 4 Normalized profiles of a Mach 7 shock wave. Conditions chosen to match those of Robben & Talbot[11], see Table I.

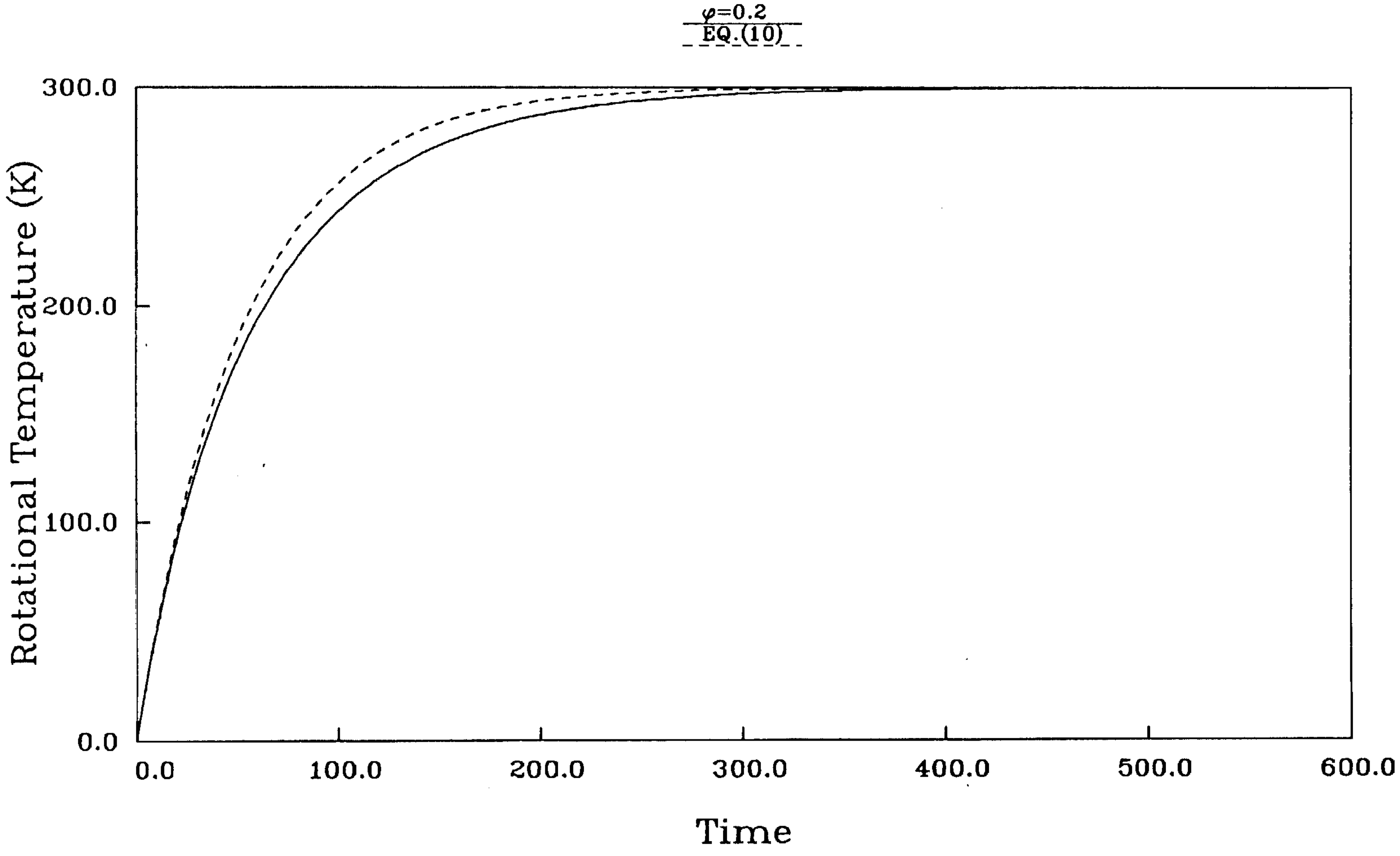
Fig. 5 Normalized density profiles of a Mach 7 shock wave for the two sets of upstream conditions investigated, see Table I.

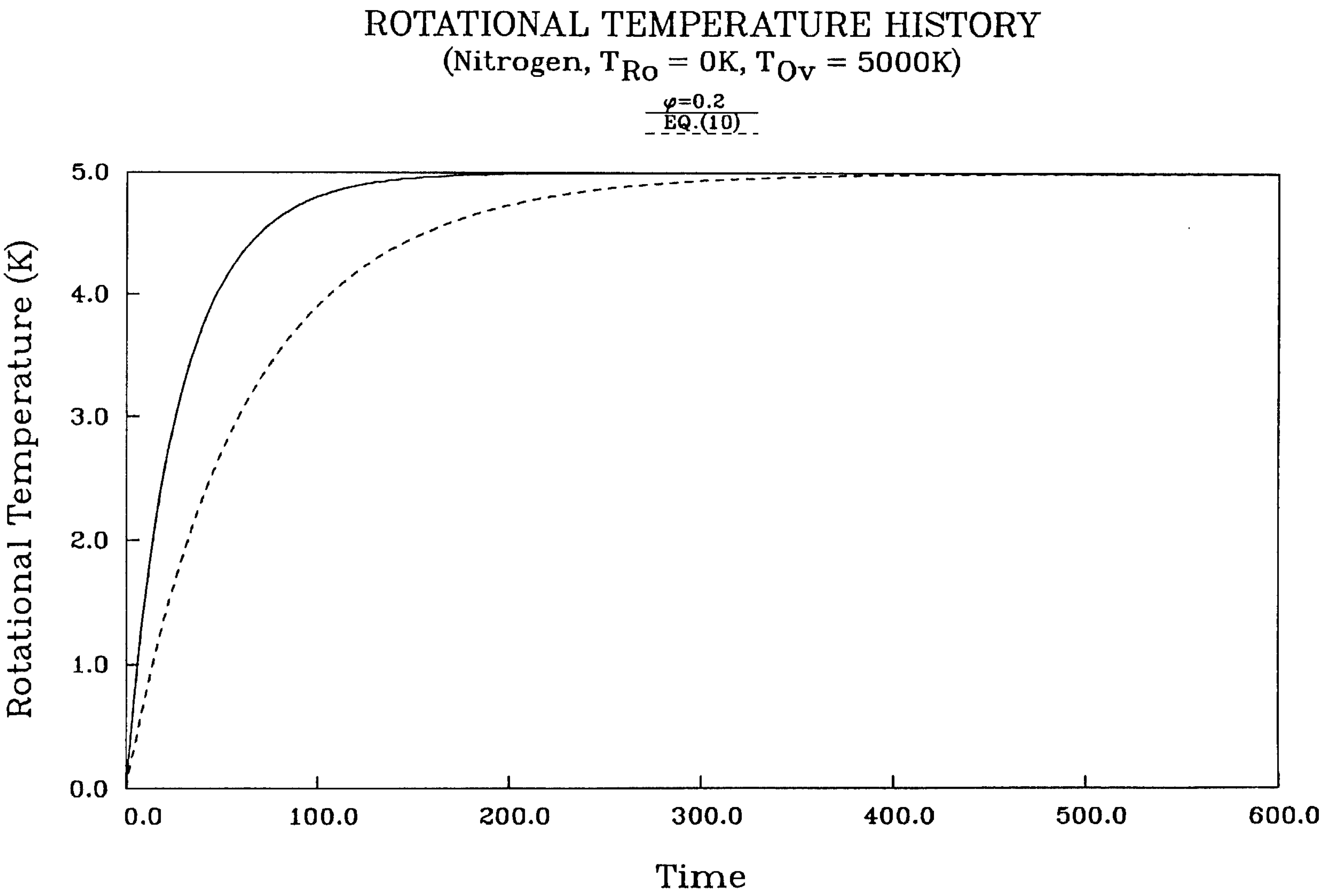
Fig. 6 Normalized temperature profiles of a Mach 7 shock wave. Upstream conditions: T_1=300K, ρ_1=7.77x10^{-3}kg m^{-3}, see Table I.


ROTATIONAL COLLISION NUMBER
Eq.(4)
□ Eq.(10)
Collision Number
25.0
20.0
15.0
10.0
5.0
0.0
0.0
500.0
1000.0
1500.0
2000.0
2500.0
3000.0
3500.0
4000.0
4500.0
5000.0
Temperature (K)

ROTATIONAL TEMPERATURE HISTORY

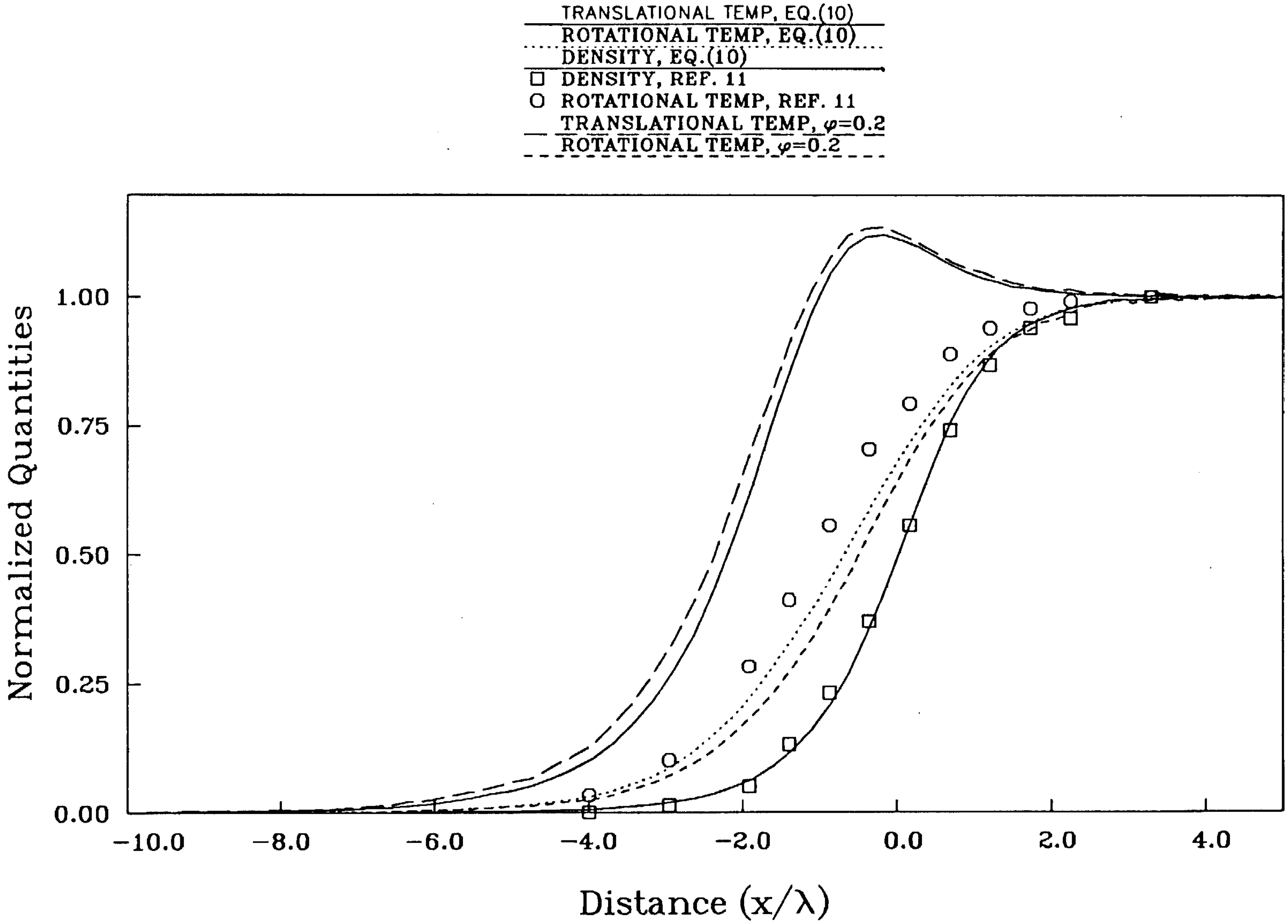
(Nitrogen, $T_{Ro} = 0K$, $T_{Ov} = 300K$)

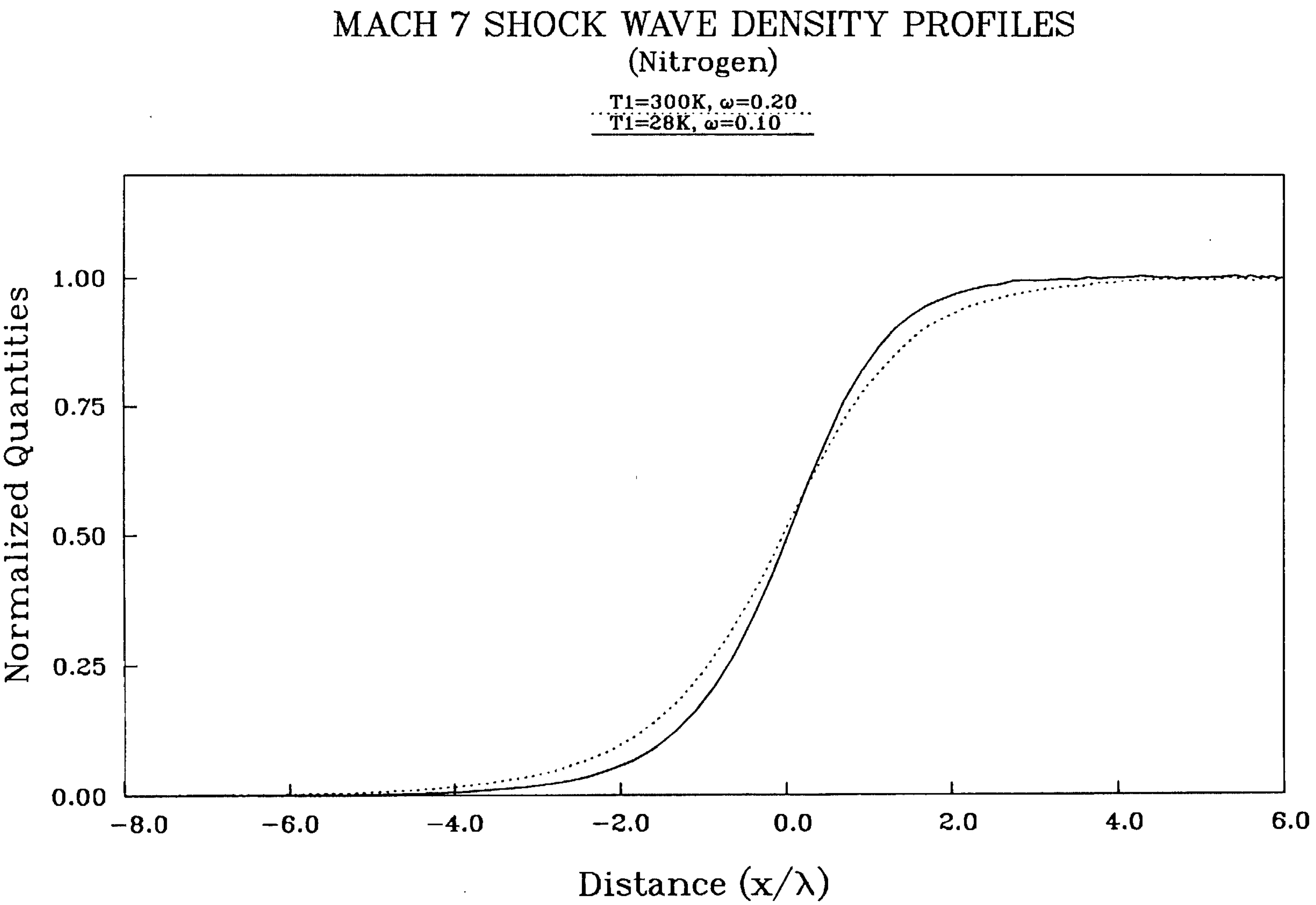



ROTATIONAL TEMPERATURE HISTORY
(Nitrogen, T_{Ro} = 0K, T_{Ov} = 5000K)
φ=0.2
EQ.(10)
Rotational Temperature (K)
0.0
1.0
2.0
3.0
4.0
5.0
0.0
100.0
200.0
300.0
400.0
500.0
600.0
Time

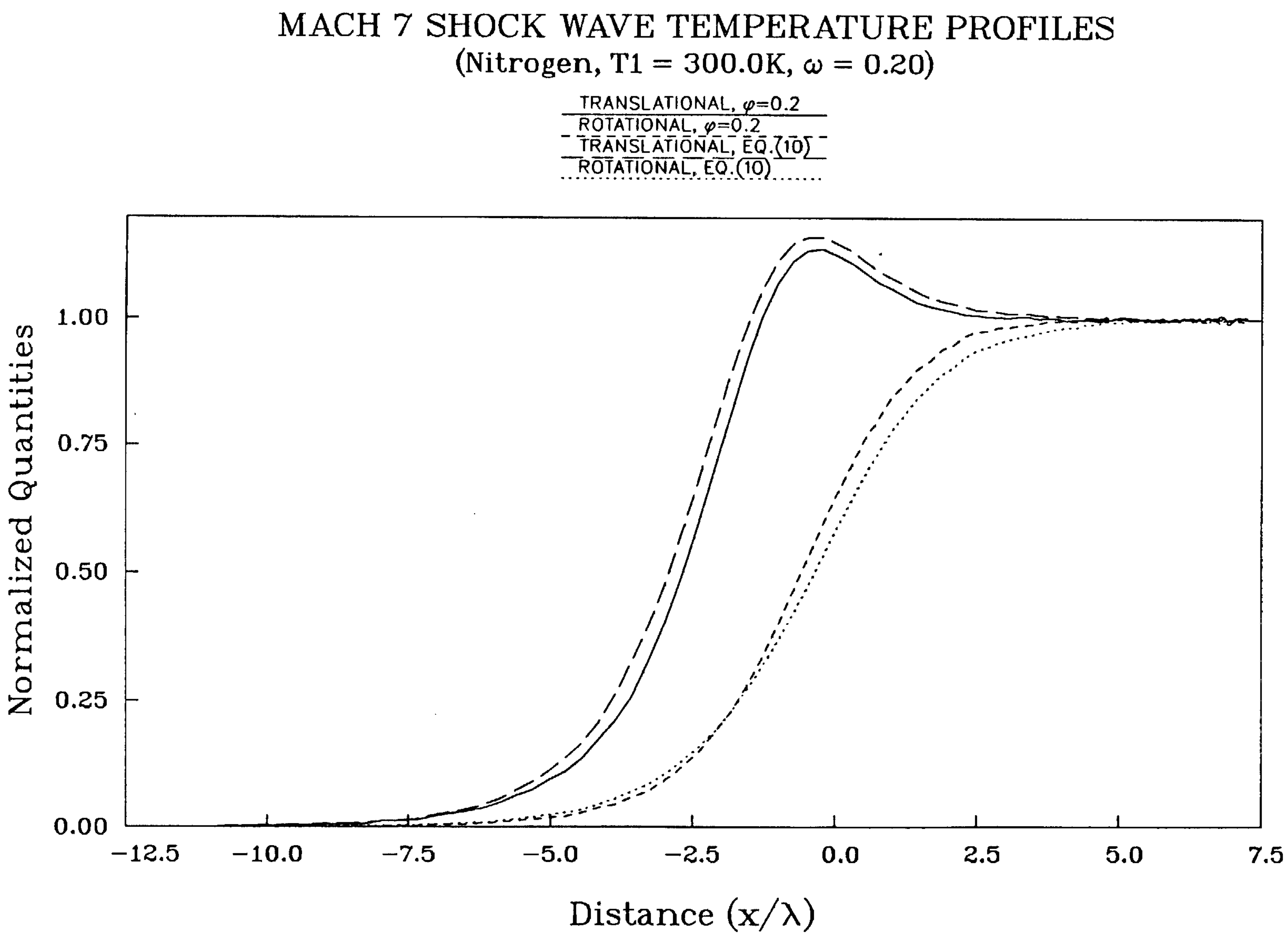
NORMALIZED MACH 7 SHOCK WAVE PROFILES

(Nitrogen, T1 = 28K, $\omega = 0.10$)





MACH 7 SHOCK WAVE DENSITY PROFILES
(Nitrogen)


MACH 7 SHOCK WAVE TEMPERATURE PROFILES
(Nitrogen, T1 = 300.0K, ω = 0.20)

APPENDIX B