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Accuracy of the Burnett Equations for Hypersonic Real Gas Flows

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The Burnett equations have long been proposed as an alternative to the Navier-Stokes equations for flows exhibiting translational nonequilibrium. However, Burnett solutions for hypersonic flows have until recently been unattainable. Burnett solutions of normal shock-wave structure are presented for four gases: two purely theoretical gases, Maxwellian and hard-sphere, and two real gases, argon and nitrogen. For the theoretical gases, solutions are obtained for Mach numbers from 1.1 to 50, and, for the real gases, solutions range from Mach 1.1 to Mach 11. These Burnett solutions are compared with Direct Simulation Monte Carlo (DSMC) solutions, with Navier-Stokes solutions, and, for the real gases, with experimental data. Experimental data and DSMC solutions represent the assumed correct solution, while Burnett and Navier-Stokes solutions represent continuum approximations. For the three monatomic gases, Burnett solutions are significantly more accurate than Navier-Stokes solutions. For nitrogen, fundamentally different solutions are obtained since rotational nonequilibrium must be included. For this diatomic case, the Burnett solutions also are more accurate than the Navier-Stokes solutions, however, best agreement between DSMC, experiment, and Burnett require different values of rotational collision number in the DSMC and Burnett simulations. The Burnett equations thus represent a significant improvement over Navier-Stokes equations for flows exhibiting translational nonequilibrium.

Nomenclature

c_{vr}, c_{vt} = rotational and translational specific heats
E = total fluid energy per unit volume
e_r, e_t = rotational translational energies per unit mass
$e_r^{eq}(T_t)$ = effective rotational energy of translation
p = $\rho R T_t$, thermodynamic pressure
Q_p = density asymmetry (shape) factor
q = one-dimensional heat flux vector
R = gas constant
T_0 = reference temperature for viscosity
T_r = rotational temperature
T_t = translational temperature
T^* = reference temperature used for Z_R
t = time
t_p = shock reciprocal thickness
u = one-dimensional fluid velocity
x_i = spatial component
Z_R = rotational collision number
Z_R^∞ = infinite temperature collision number
$\Delta_{\rho T}$ = shock density temperature separation
κ_r = μc_{vr}, rotational thermal conductivity
κ_t = $\frac{5}{2}\mu c_{vt}$, translational thermal conductivity
λ = mean free path
μ = viscosity
μ_0 = reference viscosity
ν = repulsive potential inverse power
ρ = density
σ = one-dimensional stress tensor
τ_c = $\pi\mu/4p$, mean collision time
ω = viscosity-temperature exponent
ω_i, θ_i = Burnett coefficients
ϖ, ϑ = simplified translational nonequilibrium model

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Introduction

FUTURE transatmospheric vehicles will enhance mankind's ability to operate in space. Such vehicles include ascent vehicles such as the National Aerospace Plane (NASP) and aero-braking vehicles such as Aerospace Transfer Vehicle (ASTV). Significant portions of these vehicles' flight envelopes encompass a regime known as the continuum-transition regime.

Most aerodynamicists are familiar with continuum flow where numerous collisions between molecules lead to full equilibrium. By contrast, in the continuum-transition regime there are insufficient collisions to allow the gas to come to full equilibrium giving rise to regions of nonequilibrium. Beyond the continuum-transition regime, where collisions among molecules can be neglected to a good approximation, only the collisions between molecules and solid boundaries are important. This regime is known as the free molecule or fully rarefied regime.

Theories for continuum flow and fully rarefied flow are well known. In contrast, the theory for the continuum-transition regime, which needs to bridge these two disparate theories, is not nearly as well developed. To understand these difficulties, one must begin with the Boltzmann equation which is sufficiently general in that it applies in the continuum, continuum-transition, and fully rarefied regimes. Unfortunately, it is difficult to solve for this general case, and it is therefore necessary to make approximations which cause the resulting theories to apply to limited flow regimes.

For continuum flow, it is assumed that the Knudsen number, the ratio of mean free path to some characteristic length, is small. With this assumption, a perturbation expansion of the Boltzmann equation in Knudsen number is possible. Chapman[1] and Enskog[2] independently developed such a pro-

cedure which is known today as the Chapman-Enskog expansion. The zeroth-order expansion gives the Euler equations while retaining terms up to first order yields the Navier-Stokes equations. Furthermore, the Chapman-Enskog theory determines viscosity's dependence on temperature, whereas only empirical relationships were known prior to the Chapman-Enskog theory.

The natural extension of the Chapman-Enskog theory is to carry the expansion to ever increasing powers of Knudsen number. If the expansion converges, each step results in a partial differential equation set which is applicable further into the continuum-transition regime. Burnett was the first to perform the second-order accurate Chapman-Enskog expansion, giving the equations that bear his name. Two factors have limited the acceptance of the Burnett equations. First, they are complex, making any attempt to solve or analyze them tedious. Second, and more importantly, attempts prior to 1988 to solve the Burnett equations for normal shocks with a Mach number greater than two failed.

Burnett Solution History

Checks of the accuracy of the Burnett equation for the continuum-transition regime have employed the normal shock wave as a model problem. This problem is ideal for such a check since the structure of a normal shock spans a length from four to hundreds of mean free paths depending on the chosen Mach number and gas. If this length is used to define a Knudsen number, then this Knudsen number is certainly not small, and, in fact, can approach values as high as 0.3. It can therefore be surmised that the Navier-Stokes equations will not accurately reproduce shock wave structure. Comparisons with experimental data show this to be the case. The normal shock wave also has the advantage of requiring a solution in only one dimension as well as avoiding the complications of dealing with uncertain solid-surface boundary conditions.

Early attempts to solve the Burnett equations for normal shock-wave structure centered on the set of ordinary differential equations which is valid for steady one-dimensional flow. Next, the method used by von Mises[3] and Gilbarg and Paolucci[4] to solve the similarly reduced Navier-Stokes equations was applied. Performing such a study, Talbot and Sherman[5] found that this method fails to achieve solutions above a Mach number near two, and that the attainable solutions differed only slightly from corresponding Navier-Stokes solutions. They therefore concluded "the Burnett equations make no improvement which merits the trouble of solving them."

The inability to solve the Burnett equations caused most researchers to abandon the Burnett equations and search for other methods to model flows in the continuum-transition regime. One such widely accepted method is the Direct Simulation Monte Carlo (DSMC) method initially proposed by Bird.[6] Using a much different approach, this method attempts to directly simulate rather than solve the Boltzmann equation. The DSMC method simulates the gas as a collection of thousands or millions of particles. Particles are moved in a deterministic fashion, and collisions between particles are handled statistically. Particles are periodically sampled to determine macroscopic quantities such as density and temperature. More involved sampling can determine detailed information such as the velocity distribution function; however, obtaining this microscopic information requires a much larger sample size. DSMC simulations of normal shocks agree quite well with experimental data. Pham-Van-Diep and Erwin[7] have shown that DSMC-derived velocity distributions for normal shock waves agree well with experimental measurements. Such favorable comparisons add validity to the claim of Bird[8] that DSMC simulations capture the true physics of the normal shock wave.

A disadvantage of the DSMC technique is that since macroscopic parameters are determined by statistical sampling, the error is inversely proportional to the square root of the number of samples, and hence a doubling of accuracy requires a quadrupling of computational data. Furthermore, as one approaches the continuum regime, the mean free path decreases, resulting in the need for increasingly smaller computational cells, thus leading to a rapid increase in computational effort, the net result being that accurate DSMC simulations in the continuum regime are at present prohibitively expensive, whereas solving the Navier-Stokes or Burnett equations sets does not exhibit such a cost penalty.

Recent Burnett Progress

Efforts to find efficient methods for calculating flows in the continuum-transition regime led a group of researchers at Stanford University to reevaluate the Burnett equations. This has led to a significant breakthrough—Burnett shock structure solutions for hypersonic Mach numbers.

Fiscko and Chapman[9–12] were the first to calculate hypersonic Burnett shock solutions. These solutions were obtained by abandoning the steady state equations and instead using the time-dependent equation set with modern computational fluid dynamic techniques. In this manner solutions were obtained up to Mach 50 for three types of gases: hard-sphere, argon (inverse tenth repulsive potential), and Maxwellian. Fiscko and Chapman then compared shock-wave structures computed by the DSMC method to both Navier-Stokes and Burnett solutions. In all cases the Burnett equations gave significant improvements over the Navier-Stokes equations. Fiscko and Chapman concluded that the previous failure of Burnett equations was due to the numerical method rather than the equations themselves. There was, however, a curious anomaly in this work. For the Maxwellian gas, hypersonic solutions could only be achieved for relatively coarse meshes. The reason for this anomaly is now understood and is completely documented by Zhong et al.[13] who demonstrate that the Burnett equations are in fact unstable when perturbed by a small wavelength disturbance. Refined meshes capture this disturbance and thus attempts to solve the Burnett equations on fine meshes fail. Zhong et al., further show that the Burnett equations can be stabilized by including select terms from the third-order Chapman-Enskog expansion. Since the additional terms are third order corrections, the resulting equations set is still second-order accurate. Zhong et al., in fact demonstrate that the additional terms just slightly affect shock structure solutions. Fiscko and Chapman's conclusion that choice of numerical method allows the Burnett equations to be solved is therefore only partially correct. In reality, the numerical method allowed for an underlying instability in the Burnett equation to be suppressed.

The DSMC results of Fiscko and Chapman demonstrated that the Burnett equations are more accurate than the Navier-Stokes equations for calculating normal shock-wave structure. Subsequent investigation of these DSMC results, however, discovered inaccuracies in the hard-sphere and Maxwellian results as compared with other researchers' DSMC results. The hard sphere inaccuracy was traced to an error in the isotropic scattering dictated by hard-sphere collision mechanics. This error led to a statistical bias which favored a collision velocity oriented along the flow-wise direction, resulting in shocks that were approximately 30% too thick. The inaccuracy in the Maxwellian results was traced to an inaccuracy in the curve fit of particle scattering angle as a function of impact parameter. Use of an improved fit eliminated the inaccuracy.

The work of Fiscko and Chapman dealt with monatomic gases. The application of the Burnett equations to shock waves in diatomic gases was first presented by Lumpkin and Chapman.[14,15] This work demonstrated that the Burnett equations in conjunction with a suitable model for treating rotational relaxation yields shock thicknesses which agree with experimental data. Lumpkin and Chapman also demonstrated that a simplified model could replace the Burnett equations, and still achieve significant improvements over the Navier-Stokes

equations. These improvements are however not as good as those achieved using the Burnett equations.

Goals of Current Study

This article is intended to satisfy three main goals. First, this article is intended to provide corrected and improved high-resolution DSMC results for hypersonic shocks in monatomic gases. These DSMC results will serve as a reliable test base for assessing the accuracy of various continuum equations more advanced than Navier-Stokes, such as the Burnett equations. In order to carry out this objective it is necessary to do the following:

1) Correct the error in the hard-sphere collision mechanics used to calculate the DSMC results of Fiscko and Chapman.

2) Improve the functional relationship used by Fiscko and Chapman to fit scattering angle as a function of impact parameter for the Maxwellian gas.

3) Use the best parameters to fit the available data for the argon potential energy surface to the inverse power repulsive potential model.

4) Validate the new DSMC results by comparing with other researchers' DSMC results for a few cases.

A second goal of this article is to reassess the main conclusion of Fiscko and Chapman that the Burnett equations are more accurate than the Navier-Stokes equations for all gases and all Mach numbers in matching DSMC shock-wave results. This will be done by comparing the improved and corrected DSMC results with Burnett results. The Burnett results will include the following enhancements and corrections not incorporated in the results of Fiscko and Chapman:

1) Correction of the value of the hard-sphere Burnett coefficient ω_5 from $\omega_5 = 1.428$ used by Fiscko and Chapman, to the correct value, $\omega_5 = 0.219$

2) Use of Burnett coefficients more appropriate for the assumed molecular model as opposed to Fiscko and Chapman's use of the hard-sphere or Maxwellian values [see Eq. (4) below]

Finally, this paper intends to present Burnett results for shocks in a diatomic gas, nitrogen, which includes improvements to the earlier work of Lumpkin and Chapman. These improvements are:

1) Item 2 immediately above which deals with the use of improved Burnett coefficients

2) Adjustments mentioned below to a simplified model which can be used instead of the Burnett equations

Governing Equations

The time-accurate Burnett equations in one spatial dimension are

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} = 0$$

$$\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(\rho u^2 + p) = \frac{\partial \tau}{\partial x}$$

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x}(Eu + pu) = -\frac{\partial q}{\partial x} + \frac{\partial(\tau u)}{\partial x} \tag{1}$$

where the shear stress and heat flux are given by

$$\tau = \frac{4}{3}\mu\frac{\partial u}{\partial x} - \frac{\mu^2}{p}\left[\left(\frac{2}{3}\omega_1 - \frac{14}{9}\omega_2 + \frac{2}{9}\omega_6\right)\left(\frac{\partial u}{\partial x}\right)^2 - \frac{2}{3}\omega_2\frac{kT_t}{m\rho}\frac{\partial^2 \rho}{\partial x^2} + \frac{2}{3}\omega_2\frac{kT_t}{m\rho^2}\left(\frac{\partial \rho}{\partial x}\right)^2 - \frac{2}{3}(\omega_2 - \omega_4)\cdot\frac{k}{m\rho}\frac{\partial \rho}{\partial x}\frac{\partial T_t}{\partial x} + \frac{2}{3}(\omega_4 + \omega_5)\frac{k}{mT_t}\left(\frac{\partial T_t}{\partial x}\right)^2 - \frac{2}{3}(\omega_2 - \omega_3)\frac{k}{m}\frac{\partial^2 T_t}{\partial x^2}\right]$$

$$q = -\kappa_t\frac{\partial T_t}{\partial x} + \frac{\mu^2}{\rho}\left[\left(\theta_1 + \frac{8}{3}\theta_2 + \frac{2}{3}\theta_3 + \frac{2}{3}\theta_5\right)\frac{1}{T_t}\frac{\partial u}{\partial x}\frac{\partial T_t}{\partial x} + \frac{2}{3}(\theta_2 + \theta_4)\frac{\partial^2 u}{\partial x^2} + \frac{2}{3}\theta_3\frac{1}{\rho}\frac{\partial u}{\partial x}\frac{\partial \rho}{\partial x}\right]$$

and $E = \rho(e_t + \frac{1}{2}u^2)$ is the total energy per unit volume. Note that these equations differ from the Navier-Stokes equations only in that additional terms involving second derivatives or products of first derivatives appear in the constitutive relations. Eq. (1) is not stable, as pointed out by Bobylev.[16] The following additions to stress and heat flux suggested by Zhong et al.,[13] are required to maintain stability

$$\tau_{\text{augment}} = \frac{2}{9}\frac{\mu^3}{p^2}RT_t\frac{\partial^3 u}{\partial x^3}$$

$$q_{\text{augment}} = \frac{\mu^3}{p\rho}\left\{\frac{11}{16}R\frac{\partial^3 T_t}{\partial x^3} - \frac{5}{8}\frac{RT_t}{\rho}\frac{\partial^3 \rho}{\partial x^3}\right\} \tag{2}$$

The Burnett equations are complete except for an equation of state, a relationship between viscosity and flow quantities, and the parameters ω_i and θ_i. Since the gas is not dense, the perfect gas equation of state is adequate. The viscosity relationship as well as the parameters ω_i and θ_i can be determined from Chapman-Enskog theory once a molecular model has been chosen. A simple molecular model which is accurate enough for most hypersonic calculations is the inverse power potential. Chapman-Enskog theory gives the viscosity of such a molecule as

$$\mu = \mu_0\left(\frac{T_t}{T_0}\right)^{(1/2)+2(\nu-1)} = \mu_0\left(\frac{T_t}{T_0}\right)^{\omega} \tag{3}$$

The pure numbers ω_i and θ_i must be calculated from Chapman-Enskog theory using an iterative procedure. For the general inverse power molecule only the first step in this iterative procedure, which gives an exact result for Maxwellian molecules ($\omega = 1$), has been carried out. For a hard-sphere gas ($\omega = 0.5$) three steps of the iterative process have been performed resulting in values accurate to within 0.001. The hard-sphere and Maxwellian gases are theoretical gases which can be viewed as the limiting cases for the behavior of a real gas since for almost all real gases $0.5 < \omega < 1$. Since the Burnett coefficients ω_i and θ_i are unknown for arbitrary repulsive potential, Lumpkin[15] has suggested the following interpolative scheme to approximate the Burnett coefficients as a function of viscosity-temperature exponent ω:

$$\Omega \equiv 2 - 2\omega = \begin{cases} 0, & \text{Maxwellian gas} \\ 1, & \text{hard-sphere gas} \end{cases}$$

$$\omega_1 = (1 + 0.014\Omega) \times \frac{4}{3}\left(\frac{7}{2} - \omega\right)$$

$$\omega_2 = 2 \times (1 + 0.014\Omega)$$

$$\omega_3 = 3 \times (1 - 0.194\Omega)$$

$$\omega_4 = 0 + 0.681\Omega$$

$$\omega_5 = (1 - 0.194\Omega) \times 3\omega - 0.990\Omega$$

$$\omega_6 = 8 \times (1 - 0.072\Omega)$$

$$\theta_1 = (1 + 0.035\Omega) \times \frac{15}{4}\left(\frac{7}{2} - \omega\right)$$

$$\theta_2 = -\frac{45}{8} \times (1 + 0.035\Omega)$$

$$\theta_3 = -3 \times (1 + 0.030\Omega)$$

$$\theta_4 = 3 \times (1 - 0.194\Omega)$$

$$\theta_5 = 3\left[\frac{35}{4} \times (1 - 0.082\Omega) + \omega \times (1 - 0.194\Omega) - 0.050\Omega\right] \quad (4)$$

The Burnett equations are valid for monatomic gases only. For diatomic gases some account of molecular rotation must be included. Doing this from first principles requires a form of the Boltzmann equation which accounts for molecular rotation. Carrying out the Chapman-Enskog expansion on such a version of the Boltzmann equation is more difficult than the corresponding monatomic case. One must decide whether to carry the expansion out using a single temperature to describe all energy modes or to instead use separate temperatures for rotation and translation. Making this choice requires some knowledge of the mechanism of rotational-translational energy transfer. If the exchange occurs freely, then rotation and translation will be nearly equilibrated justifying the use of a single temperature. However, if energy exchange is restricted, then large amounts of rotational nonequilibrium can occur. Wang Chang and Uhlenbeck[17] were the first to carry out the Chapman-Enskog expansion to first order for such a system, and found that for easy exchange the presence of rotation is manifested by an additional bulk viscosity. Wang Chang and Uhlenbeck also studied the case of difficult exchange and found that the Chapman-Enskog expansion to first order for such a system yields the Navier-Stokes equations with total energy per unit volume $E = \rho(e_r + e_t + \frac{1}{2}u^2)$ plus the following additional equation describing the time evolution of rotational energy

$$\rho \frac{De_r}{Dt} - \frac{\partial}{\partial x_i} \kappa_r \frac{\partial T_r}{\partial x_i} = \rho \frac{e_r^{eq}(T_t) - e_r}{Z_R \tau_c} \quad (5)$$

This equation is the substantial derivative form of Jeans's equation[18] describing the time evolution of rotational energy in a gas of slightly loaded spheres, the simplest classical model for a diatomic gas. The term "slightly" refers to an assumption made in Jeans's derivation and corresponds to the case of difficult energy exchange between rotation and translation. The form of Eq. (5) is also identical to the Landau-Teller[19] equation for relaxation of a gas of harmonic oscillators. Since the Landau-Teller equation applies to vibrational nonequilibrium, whereas Jeans's equation is intended for rotational nonequilibrium, we will refer to Eq. (5) as Jeans's equation throughout.

The value Z_R is known as the rotational collision number. Parker[20] suggested the following function form for Z_R on the basis of a two-dimensional scattering computation

$$Z_R = \frac{Z_R^\infty}{1.0 + \frac{\pi^{3/2}}{2}\left(\frac{T^*}{T_t}\right)^{1/2} + \left(\frac{\pi^2}{4} + \pi\right)\left(\frac{T^*}{T_t}\right)} \quad (6)$$

Lordi and Mates[21] have validated the general form of the Parker expression for collisions occurring in three dimensions; however, slightly different values of Z_R^∞ and T^* from those suggested by Parker are needed. Parker suggested using $Z_R^\infty = 15.7$ and $T^* = 80$ K, whereas the Lordi and Mates computations are better fit by $Z_R^\infty = 23.0$ and $T^* = 91.5$ K.

To our knowledge, no one has carried out the Chapman-Enskog expansion to Burnett level for a gas possessing rotational energy. However, Lumpkin and Chapman[14,15] have shown that one can use the Burnett equations in conjunction with Jeans's equation and obtain reasonably good results for shock waves in nitrogen. Additional studies by Lumpkin and Chapman[14] attempting to derive an expression for rotational relaxation which is more general than Jeans's equation have found that for a shock wave in nitrogen Jeans's equation is probably a good approximation to the true physics.

Lumpkin and Chapman[14] also demonstrate that the key features of the Burnett equations can be captured by a much simpler model. This model has been named the simplified translational nonequilibrium model (STNM). It has been slightly modified since its original presentation. The modification is due to a decision to model argon with an inverse ninth molecular potential rather than an inverse tenth. It is felt that this value of ν more accurately represents the majority of published viscosity-temperature data for argon. The stress and heat flux for the STNM are

$$\tau = \frac{4}{3}\mu \frac{\partial u}{\partial x} - \varpi \frac{\mu^2}{p}\left(\frac{\partial u}{\partial x}\right)^2 \quad (7a)$$

$$q = -\kappa_t \frac{\partial T_t}{\partial x} + \vartheta \frac{\mu^2}{\rho T_t}\left(\frac{\partial u}{\partial x}\right)\left(\frac{\partial T_t}{\partial x}\right) \quad (7b)$$

where

$$\varpi = 8, \quad \vartheta = \left(\theta_1 + \frac{8}{3}\theta_2 + \frac{2}{3}\theta_3 + \frac{2}{3}\theta_5\right)$$

The constant ϖ, which has been reduced from 9.5 to 8, differs from the previously published model. It should also be noted that the coefficient ϑ now exactly matches the Burnett coefficient for arbitrary inverse power potential. Previously, it matched the Maxwellian value.

Numerical Methods for Shock Structure

As mentioned above, since one is only concerned with the steady shock solution, one can delete the temporal derivatives from the governing equations and then solve using ordinary differential equation solvers. This technique, however, requires an analysis of the two singularity points far upstream and downstream of the shock to determine which direction to march the solution. Marching in the proper direction maintains the solution of the correct integral curve joining the two singularities. For the Navier-Stokes equations, this proper direction is from downstream to upstream as was first demonstrated by von Mises.[3] However, if the same technique is applied to the Navier-Stokes equations in conjunction with Jeans's equation then neither direction is a stable marching direction as was pointed out by Talbot and Scala.[22] Also, if the same technique is applied to the Burnett equations then neither direction provides a stable integration path for Mach numbers greater than about 2.0. So, while using an ordinary differential equation solver to obtain the steady solutions of Eq. (1) appears attractive, in practice it can only be applied to cases where rotational energy is not present and for cases using the Navier-Stokes or STNM constitutive relations.

For any other cases, the technique used in this study time marches arbitrary initial conditions to the steady state solution. It is a hybrid implicit-explicit technique based on the predictor-corrector technique of MacCormack[23] which differs from the purely explicit MacCormack technique by implicitly treating the constitutive relations. This reduces the number of time steps required to reach steady state. In fact, implicit treatment of the Euler terms would further increase solver performance; however, this requires a technique such as flux vector splitting which introduces significant dissipation at sonic points. This is unacceptable since a shock macroscopic parameter calculated in this study, namely shock reciprocal thickness, is sensitive to smooth solutions near the sonic point. Details of this numerical procedure can be found in Lumpkin[15] and Fiscko.[12]

The DSMC results (see Table 1) are calculated using the technique outlined by Bird.[6] The inaccuracies in the Fiscko

Table 1 Various DSMC results for parameters in a Mach 11 shock in a hard-sphere gas

Researcher	λ_1/t_ρ	$\Delta_{\rho T}$	Q_ρ
Bird[24]	0.433	1.42	1.14
Boyd[25]	0.435	1.44	1.18
McDonald[26]	0.443	1.40	1.19
"Corrected" Fiscko	0.438	1.46	1.18
Fiscko[12]	0.363	1.92	1.27

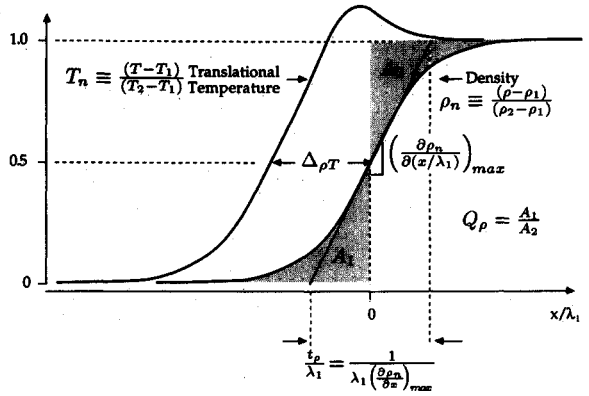

Fig. 1 Illustration of shock macroscopic parameters—shock thickness, density asymmetry, and temperature-density separation.

results mentioned above have been corrected. To check the accuracy of the corrected Fiscko results, a comparison was made with DSMC results provided by other researchers. Table 1 shows the results of this comparison for Mach 11. As can be seen, the "corrected" Fiscko results now agree within an acceptable scatter to the DSMC results of other researchers.

Results and Discussion

Navier-Stokes, Burnett, and DSMC solutions were calculated for three monatomic gases: hard-sphere, argon, and Maxwellian. Argon is now modeled with $\nu = 9$ as opposed to the value $\nu = 10$ employed by Fiscko and Chapman. Navier-Stokes and Burnett solutions for the two theoretical gases (hard-sphere and Maxwellian) were calculated for 20 Mach numbers from 1.1 to 50. For argon, the same Mach number set was used up to Mach 11. DSMC simulations were carried out for 14 Mach numbers from 1.5 to 50 for the theoretical gases, and using the same set for argon up to Mach 11. The Navier-Stokes solutions were calculated with a Runge-Kutta solver using 4000 grid points. The Burnett solutions incorporate 500 grid points and were calculated using the hybrid scheme mentioned in the previous section. The DSMC simulations use 200 cells with approximately 190 particles per cell. A large sample size was obtained by time averaging for roughly 10,000 time steps. Thus, on average, the DSMC simulations have a sample size of 2×10^6 per cell.

Important macroscopic shock parameters are illustrated in Fig. 1, namely shock reciprocal thickness λ/t_ρ, shape factor Q_ρ, and density-temperature separation $\Delta_{\rho T}$. These parameters quantify changes in shock profiles due to Mach number as well as point out subtle differences in the results from various theories.

Figures 2–4 compare temperature and density profiles for a Mach 11 shock in the hard-sphere, argon, and Maxwellian gases, respectively. Each figure compares the Navier-Stokes, Burnett, and DSMC results. It can easily be seen for all three gases the Burnett results agree much more closely with the DSMC results than do the Navier-Stokes results. Similar results were found for all Mach numbers tested. This is demonstrated in Figs. 5 and 6 which, for the two theoretical gases, show the results obtained for shock reciprocal thickness, and density-temperature separation, respectively. Again each figure compares Navier-Stokes, Burnett, and DSMC results, and

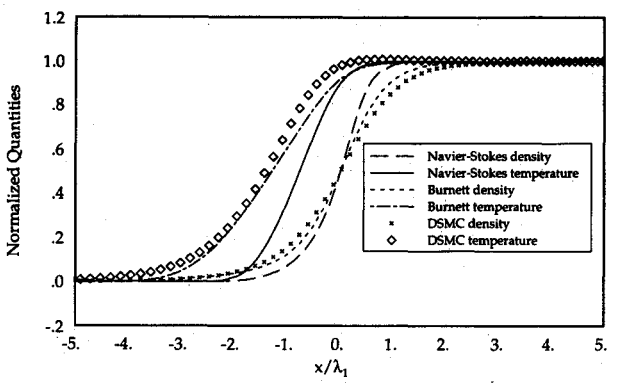

Fig. 2 Density and temperature profiles in a Mach 11 shock in a hard-sphere gas ($\nu = \infty$).

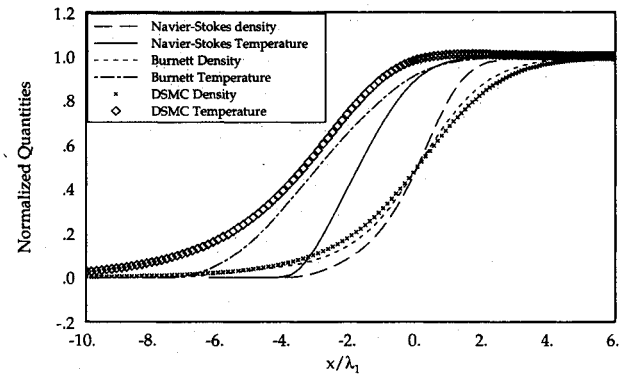

Fig. 3 Density and temperature profiles in a Mach 11 shock in argon ($\nu = 9$).

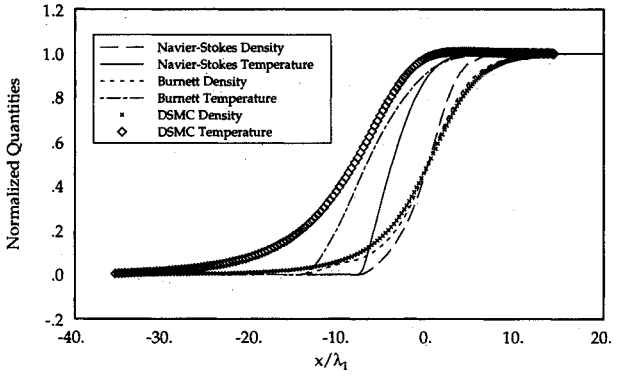

Fig. 4 Density and temperature profiles in a Mach 11 shock in a Maxwellian gas ($\nu = 5$).

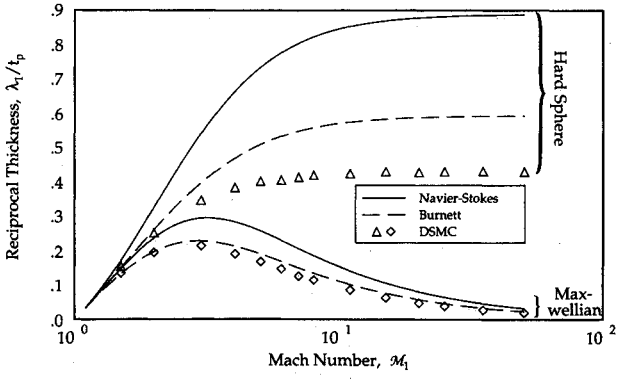

Fig. 5 Reciprocal thickness as a function of Mach number for two theoretical monatomic gases.

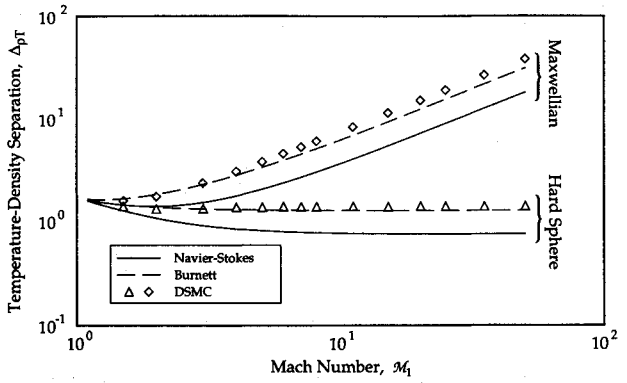

Fig. 6 Density-temperature separation as a function of Mach number of two theoretical monatomic gases.

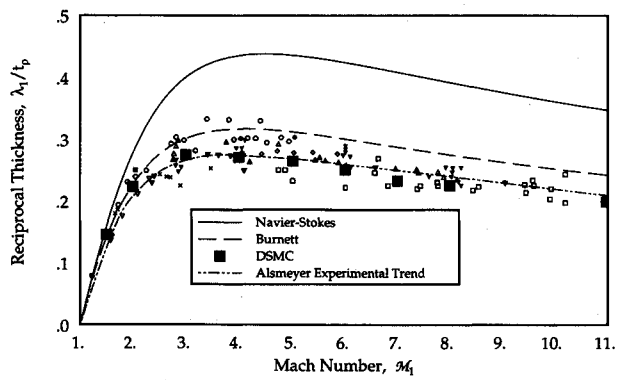

Fig. 7 Reciprocal thickness as a function of Mach number for argon (ν = 9). Small symbols represent various experimental results as compiled by Alsmeyer.

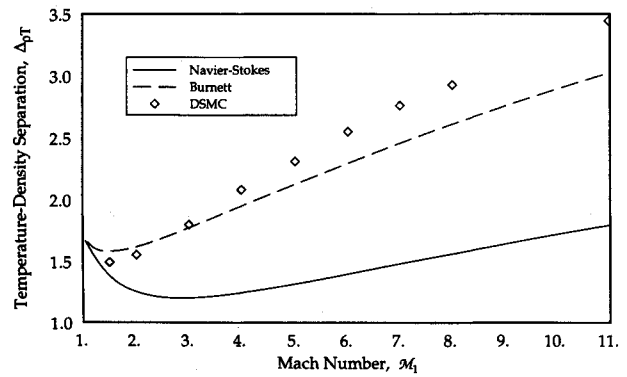

Fig. 8 Density-temperature separation as a function of Mach number for argon (ν = 9).

again it can be seen that the Burnett results are in much closer agreement to DSMC results than are the Navier-Stokes results. In fact, for the hard-sphere gas, the agreement is much better than was initially reported by Fiscko and Chapman. The DSMC results for Maxwellian gas reported herein are slightly thicker than those of Fiscko and Chapman causing the comparison of reciprocal thickness between DSMC and Burnett for this gas to yield slightly poorer agreement than was initially reported by Fiscko and Chapman. However, since this increase in the thickness of the DSMC results also degrades the "amount of agreement" for the Navier-Stokes results, the overall trend initially reported by Fiscko and Chapman is still valid.

For argon, a large body of experimental measurements of shock density profiles exists. Perhaps the most complete and accurate set of experimental data is due to Alsmeyer.[27] Figure 7 compares Alsmeyer's shock reciprocal thicknesses with DSMC, Burnett, and Navier-Stokes results. Figure 8 compares DSMC, Burnett, and Navier-Stokes values for density-temperature separation. As can be seen the Burnett results are in better agreement with both experimental and DSMC results than are the Navier-Stokes results.

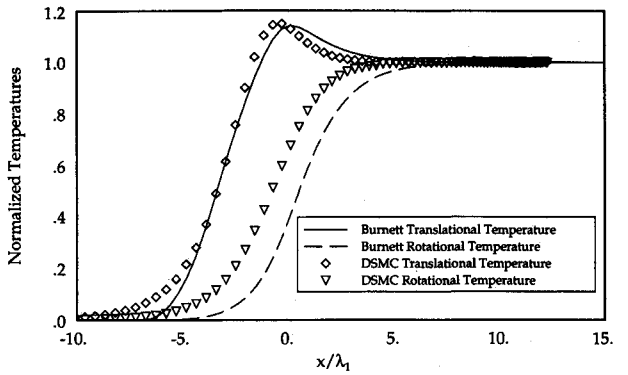

Fig. 9 Temperature profiles in a Mach 11 shock for nitrogen (ν = 10).

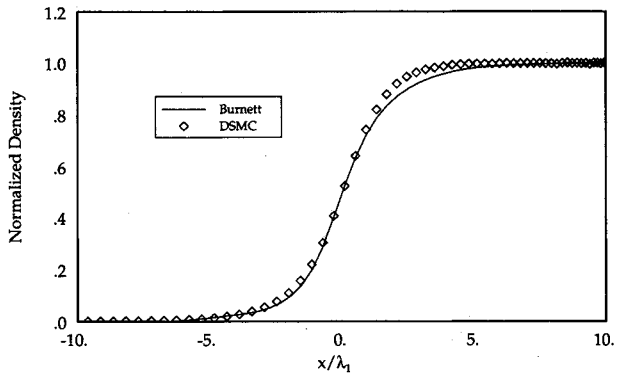

Fig. 10 Density profiles in a Mach 11 shock for nitrogen (ν = 10).

This paper concludes with results calculated for nitrogen shock waves. Here the emphasis is on demonstrating the capability of using the Burnett equations to calculate shocks in a diatomic gas rather than showing detailed comparisons. This is done for two reasons. First, once rotational nonequilibrium is present it is difficult to separate its effects from those of translational nonequilibrium, and thus the value of such a comparison is less clear. Second, for the DSMC method to account for rotational relaxation, some phenomenological model must be incorporated to account for energy exchange between rotation and translation. At present, the most popular model is the Borgnakke and Larsen[28] model which is computationally efficient and which duplicates the behavior of Jeans's equation for the case of stationary relaxation. Use of a phenomenological model is at present necessary since the actual energy exchange mechanism between rotation and translation is poorly understood. This unfortunate situation implies that DSMC simulations for a diatomic gas can no longer be thought of as adhering to first principles as is the case for a monatomic gas.

Burnett solutions for nitrogen are calculated for the Mach number set mentioned above for argon. These solutions incorporate Jeans's equation to model rotational relaxation using Parker's equation for Z_R with Z_R^∞ = 18 and T^* = 91.5K. For a Mach 11 shock this gives a range of $4.2 < Z_R < 13.5$. An inverse tenth power molecular model has been used to model nitrogen. These solutions differ from those previously reported by Lumpkin and Chapman in that they incorporate the interpolated values of the Burnett equations and the use of the stability augmentation terms allows for solutions with 500 grid points. In addition, STNM results for nitrogen are presented which incorporate the same rotational relaxation model as do the Burnett results. They differ from the earlier results of Lumpkin and Chapman in that the STNM model is now slightly modified as mentioned above.

Figure 9 gives Burnett translational temperature and rotational temperature profiles in nitrogen for a Mach 11 shock and compares them with DSMC results calculated using a computer code provided by Bird.[24] These DSMC computations use Z_R^{DSMC} = 5 in conjunction with the Borgnakke-Larsen model. Figure 10 similarly compares density profiles.

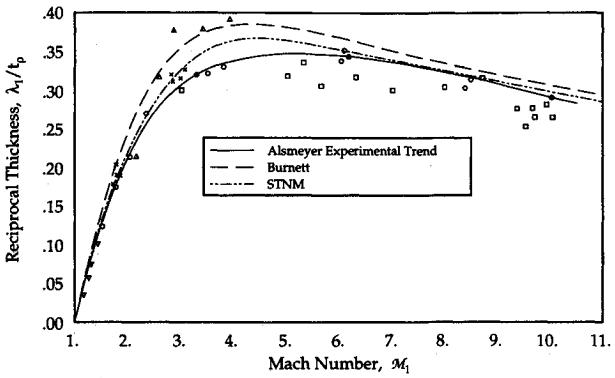

Fig. 11 Reciprocal thickness as a function of Mach number in nitrogen ($\nu = 10$). Small symbols represent various experimental results as compiled by Alsmeyer.

It is interesting to note that DSMC computations using a constant value of rotational collision number closely match Burnett results using a value which is increasing as a function of temperature. Use of Parker's model for an increasing Z_R with temperature has been incorporated into the DSMC method by Boyd.[29] This study however found it necessary to use $\omega = 0.62$ rather than $\omega = 0.72$ in order to achieve good agreement with experimental results for reciprocal thickness. This behavior is not understood at present and requires further study to resolve. Figure 11 compares experimental shock reciprocal thicknesses for nitrogen with those computed using both the Burnett equations and the STNM. In both cases the agreement is good; however, since comparisons with DSMC results for these diatomic cases is at present inconclusive, it would be desirable to have additional experimental data, such as temperature profiles, for comparison.

Conclusions

Comparisons between Navier-Stokes, Burnett, and DSMC solutions for shock structure in three monatomic gases (hard-sphere, argon, and Maxwellian) originally presented by Fiscko and Chapman have been reevaluated because of known errors and inaccuracies in the original comparisons. It has been found that resolving these issues does not alter the main conclusion originally reached by Fiscko and Chapman, namely: *For all (monatomic) gases tested and at all Mach numbers tested, the Burnett equations give an improvement over the Navier-Stokes equations as compared with DSMC and available experimental results.*

Also, the Burnett equations as well as the simplified translational nonequilibrium model have been applied to shock wave structures in diatomic gases. In both cases rotational relaxation is modeled using Jeans's equation in conjunction with Parker's equation for Z_R. These results are similar to results initially presented by Lumpkin and Chapman; however, they incorporate refinements to the previous work. These refinements have only a modest effect and thus the previous conclusion of Lumpkin and Chapman that the Burnett equations can be used in conjunction with Jeans's equation to model shock wave structure in a diatomic gas is still valid. Finally, it has been shown that in a diatomic gas the Burnett equations and the DSMC simulations require different values of rotational collision number for the results to achieve the same level of agreement as is found in monatomic gases. This result is not understood and is a subject of continuing interest.

Acknowledgments

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