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The equations describing the physical properties of a gaseous mixture of Maxwell molecules, obtained by Walker using Grad's 13-Moment Approximation, are used to develop a set of equations for studying relaxation processes in a binary mixture. The resulting equations are transformed into a dimensionless form and solved numerically. The solutions are plotted for two cases. In the colliding gas case, the values of the dimensionless variables are plotted as functions of the self-collision number for one kind of molecule for different mass ratios. For the case of the mixture moving in one direction, the results are plotted in the form of relaxation ratios as a function of mass ratios for two different densities. In both cases, the graphs are a successful representation of the expected results.

RELAXATION IN A BINARY GASEOUS MIXTURE

OF MAXWELL MOLECULES

by

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I. INTRODUCTION

Over the years, much work has been done in developing sets of equations describing the physical properties of gaseous mixtures. One person to do such work was Walker[1], who developed a set of equations for a gaseous mixture of Maxwell molecules. His theory is valid for gases having arbitrary velocity and temperature differences but small stresses and heat fluxes.[1] Since the proposal of his equations, there has been no attempt made to solve these equations numerically. One purpose, then, of this paper is to offer numerical solutions to a dimensionless form of Walker's equations for the case of a binary gas mixture. Another purpose is to verify a qualitative prediction by Morse[2] as to what a solution of this type might reveal. His prediction is that when a gaseous mixture of a light and heavy gas is initially far from equilibrium, it will relax in three stages. In the first stage, the lighter gas molecules will relax with one another. In the second stage, the heavier molecules will equilibrate, and in the third stage, through cross-collisions, the lighter molecules and the heavier molecules will reach equilibrium with one another. This is because the relaxation time is directly proportional to the square root of the mass of the molecules in the gas.

In Sec. II, the method of obtaining Walker's equations in dimensionless form and analytic solutions to the first four of those equations is presented. A discussion of the numerical solution to the remaining four equations is given in Sec. III, and a program listing is given in the Appendix. The solution method used is a numerical integration process for solving a system of first-order ordinary differential equations known as Hamming's modified predictor-corrector method.[3] The solutions are plotted for the cases of colliding gases and gases moving in the same direction. In Sec. IV, a discussion of the results is given.

II. THE DEVELOPMENT OF DIMENSIONLESS EQUATIONS DESCRIBING A RELAXING BINARY GAS IN ONE DIMENSION

A volume element of a binary gas in equilibrium may be described microscopically in terms of a Maxwellian distribution function for each type of molecule. The physical properties of the mixture, which are constant in space and time, can be determined from these Maxwellian distributions. If the gas is not in equilibrium, it may be described by non-Maxwellian distribution functions. The physical properties of the gas in this case are determined by these distribution functions and are not constant in time and space. If left alone, a non-equilibrium gas will relax to an equilibrium Maxwellian gas.

Let us consider a non-equiilbrium gas composed of one type of molecule. The physical properties of this gas are its density n, pressure p, and temperature T. These properties are functions of position $\vec{r}$ and time t. Aside from these, further properties are needed to describe the motion, internal stresses, and flow of heat of the gas. Thr first property is the flow or drift velocity denoted by $\langle\vec{v}\rangle$ or $\vec{u}$. It is the velocity at time t of a small volume element of the gas, $d\vec{r}$, located at position $\vec{r}$. The second is the pressure or stress tensor whose elements are denoted by P_{ij}. It is a three by three matrix which basically describes the rate at which momentum is transported across an arbitrary plane in the gas. The third is the heat flux vector denoted by $\vec{q}$. It is the amount of heat crossing a plane perpendicular to $\vec{q}$ per unit time per unit area. These physical properties of the gas can be expressed in terms of a distribution function $f(\vec{r},\vec{v},t)$ such that $f(\vec{r},\vec{v},t)d\vec{r}\,d\vec{v}$ is the number of molecules located between $\vec{r}$ and $\vec{r} + d\vec{r}$ that have velocities between $\vec{v}$ and $\vec{v} + d\vec{v}$. In terms of the "moments" of this distribution function, one may define the physical properties of the gas.[1] The density is defined as

$$n(\vec{r},t) = \int f(\vec{r},\vec{v},t)\,d\vec{v} \;,$$

where the integration is performed over all velocity space.* The flow velocity is

$$\vec{u}(\vec{r},t) = \frac{1}{n}\int \vec{v}\; f(\vec{r},\vec{v},t)\,d\vec{v} = \langle \vec{v} \rangle \;.$$

The temperature T is defined by the following:

$$\frac{3}{2}kT(\vec{r},t) = \frac{1}{n}\int \frac{1}{2}ms^2 f(\vec{r},\vec{v},t)\,d\vec{v} = \left\langle \frac{1}{2}ms^2 \right\rangle \;,$$

where $\vec{s}(\vec{r},t) = \vec{v} - \vec{u}(\vec{r},t)$, is sometimes called the "perculiar" or "thermal" velocity. It is a measure of the deviation of the molecular velocity from the average molecular velocity, and k is the Boltzmann constant. The pressure tensor is described in component form. Let

$$p_{ij}(\vec{r},t) = \int m s_i s_j f(\vec{r},\vec{v},t)\,d\vec{v} = n\langle m s_i s_j \rangle \;.$$

Therefore, we can write

$$\sum_i p_{ii} = \sum_i \int m s_i s_j f(\vec{r},\vec{v},t)\,d\vec{v} = \int m s^2 f(\vec{r},\vec{v},t)\,d\vec{v} = n\langle ms^2 \rangle = 3nkT = 3p$$

where $p = nkT$ is the scalar or ordinary pressure of the gas. The

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*All integration unless otherwise stated is over the entire range of the variable of integration.

pressure tensor elements, P_{ij}, are then defined as

$$P_{ij} = nm\langle s_i s_j - \frac{1}{3} s^2 \delta_{ij} \rangle ,$$

where δ_{ij} is the Kronecker delta whose definition is

$$\delta_{ij} = \begin{cases} 1, & i = j \\ 0, & \text{otherwise.} \end{cases}$$

The heat flux vector, **q**(r,t) is defined as

$$\vec{q}(\vec{r},t) = \int \vec{s}\,\frac{1}{2} m s^2 f(\vec{r},\vec{v},t)\,d\vec{v} = n\langle \vec{s}\,\tfrac{1}{2} m s^2 \rangle .$$

The non-equilibrium properties of the gas can be completely determined, using the above definitions, from a knowledge of the distribution function $f(\vec{r},\vec{v},t)$. The basic equation used to determine the distribution function is called the Boltzmann Transport Equation. Since this equation is a very complex integro-differential equation, no exact analytic solution is known to exist. Various approximation schemes for a solution have, however, been proposed. The moment equations used in this paper were obtained by Walker[1] using Grad's 13-Moment Approximation. The adaptations imposed on those equations for use here are that no internal energies or heat fluxes are considered, and that the moments are uniform in position and vary only in time. With these restrictions, the moment equations to be considered for type "a" molecules are:

momentum,

$$m_a n_a \frac{d}{dt}(u_i)_a = \sum_b \left[\Delta(m u_i)\right]_{ab} \quad ; \tag{1}$$

translational energy,

$$\frac{3}{2} n_a k \frac{dT_a}{dt} = \sum_b \left[\Delta\left(\tfrac{1}{2} m s^2\right)\right]_{ab} \quad ; \tag{2}$$

viscous stress,

$$\frac{d}{dt}(P_{ij})_a = \sum_b \left[\Delta m(s_i s_j - \tfrac{1}{3}\delta_{ij} s^2)\right]_{ab} \quad ; \tag{3}$$

translational heat flux,

$$\frac{d}{dt}(q_i)_a = \sum_b \left[\Delta (s_i \tfrac{1}{2} m s^2)\right]_{ab} \quad ; \tag{4}$$

where the summations are over all the type molecules in the mixture and the subscripts i and j go from one to three. The right hand sides of these equations represent the collision integrals of the Boltzmann operator. Expressions for these collision integrals are given by Walker and Tanenbaum for the special case of Maxwell molecules which interact by means of an inverse fifth power central force.[4] These expressions are:

momentum,

$$\left[\Delta(m u_i)\right]_{ab} = n_a \nu_{ab} \mu (\vec{u}_b - \vec{u}_a) \quad ; \tag{5}$$

translational energy,

$$\left[\Delta(\tfrac{1}{2} m s^2)\right]_{ab} = 2 n_a \nu_{ab} x y \left[\tfrac{3}{2} k (T_b - T_a) + \tfrac{1}{2} m_b (\vec{u}_b - \vec{u}_a)^2\right] ; \tag{6}$$

viscous stress,

$$\left[\Delta m(s_i s_j - \tfrac{1}{3}\delta_{ij} s^2)\right]_{ab} = 2\beta m_a n_a \nu_{ab} y^2 \Big[(1 - \beta^{-1} y^{-1}) \frac{P_{aij}}{m_a n_a}$$

$$+ \frac{P_{bij}}{m_b n_b} + (u_{bi} - u_{ai})(u_{bj} - u_{aj}) - \tfrac{1}{3}\delta_{ij}(\vec{u}_b - \vec{u}_a)^2\Big] \quad ; \tag{7}$$

translational heat flux,

$$\left[\Delta(\tfrac{1}{2} m_a s_a^2 s_{ai})\right]_{ab} = 2 m_a n_a \nu_{ab} \left(\frac{m_b}{m_a + m_b}\right)^3 \left\{\frac{q_{bi}}{m_b n_b} - \left[\gamma - (1-\gamma)\left(\frac{m_b}{m_a + m_b}\right)^{-1}\right.\right.$$

$$+\frac{3}{2}\left(\frac{m_b}{m_a+m_b}\right)^3\Bigg]\frac{q_{ai}}{m_a n_a} + \Delta_j \gamma \frac{P_{bji}}{m_b n_a} + \Delta_j \frac{P_{aji}}{m_a n_a}\left[\gamma - \left(\frac{1}{4}\gamma + \frac{3}{2}\right)\left(\frac{m_b}{m_a+m_b}\right)^{-1}\right.$$

$$\left. + \frac{1}{2}\left(\frac{m_b}{m_a+m_b}\right)^{-2}\right] + \frac{1}{2}\Delta_i\left[\gamma\Delta^2 + 5\gamma\left(\frac{k}{m_b}\right)(T_b - T_a) + \left(\frac{5k(m_a+m_b)}{24 m_b}\right)T_a\right]\Bigg\} \quad (8) \;;$$

where a and b denote a particular pair of molecules, $\mu = m_a m_b/(m_a + m_b)$, $x = m_a/(m_a + m_b)$, $y = m_b/(m_a + m_b)$, $\Delta = u_a - u_b$, $\beta \cong 0.225$, $\gamma \cong 0.968$, and ν_{ab} is the cross collision frequency given by $\nu_{ab} = 2\pi A_1(5)(K_{ab}/\mu)^{\frac{1}{2}} n_b$, with $A_1(5)$ being the dimensionless collision cross section, and K_{ab} being the interparticle force constant.[4] Substituting these collision terms, equations(5) - (8), into the right hand side of eauations (1) - (4) and considering only a one dimensional binary gas of type 1 and 2 molecules, the equations describing the gas become:

momentum,

$$\frac{du_1}{dt} = \nu_{12}\frac{m_2}{m_1+m_2}(u_2 - u_1) \quad , \qquad (9)$$

$$\frac{du_2}{dt} = -\nu_{21}\frac{m_1}{m_1+m_2}(u_2 - u_1) \quad ; \qquad (10)$$

translational energy,

$$\frac{3}{2}k\frac{dT_1}{dt} = 2\nu_{12}\frac{m_1 m_2}{(m_1+m_2)^2}\left[\frac{3}{2}k(T_2 - T_1) + \frac{1}{2}m_2(u_2 - u_1)^2\right], \qquad (11)$$

$$\frac{3}{2}k\frac{dT_2}{dt} = 2\nu_{21}\frac{m_1 m_2}{(m_1+m_2)^2}\left[-\frac{3}{2}k(T_2 - T_1) + \frac{1}{2}m_1(u_2 - u_1)^2\right]; \qquad (12)$$

viscous stress,

$$\frac{dP_1}{dt} = \nu_{11}(\beta - 1)P_1 + 2\beta\mu_{12}\left(\frac{m_2}{m_1+m_2}\right)^2\left[\left(1 - \frac{m_1+m_2}{\beta m_2}\right)P_1 + P_2\frac{n_1}{n_2}\frac{m_1}{m_2}\right.$$

$$+ \frac{2}{3} m_1 n_1 (u_2-u_1)^2 \Big] , \tag{13}$$

$$\frac{dP_2}{dt} = \nu_{22}(\beta-1)P_2 + 2\beta\nu_{21}\left(\frac{m_1}{m_1+m_2}\right)^2\Big[\left(1-\frac{m_1+m_2}{\beta m_1}\right)P_2 + P_1\frac{n_2}{n_1}\frac{m_2}{m_1}$$

$$+\frac{2}{3} m_2 n_2 (u_2-u_1)^2\Big] ; \tag{14}$$

translational heat flux,

$$\frac{dq_1}{dt} = \frac{1}{4}\nu_{11}(\gamma-3)q_1 + 2\nu_{12}\left(\frac{m_2}{m_1+m_2}\right)^3\Big\{q_2\frac{m_1}{m_2}\frac{n_1}{n_2} - \Big[\gamma-(1+\gamma)\left(\frac{m_1+m_2}{m_2}\right)+\frac{3}{2}\left(\frac{m_1+m_2}{m_2}\right)\Big]q_1$$

$$+\frac{m_1}{m_2}\frac{n_1}{n_2}(u_2-u_1)P_2 + P_1(u_2-u_1)\Big[\gamma-\left(\frac{1}{4}\gamma+\frac{3}{2}\right)\left(\frac{m_1+m_2}{m_2}\right)+\frac{1}{2}\left(\frac{m_1+m_2}{m_2}\right)^2\Big]$$

$$+\frac{1}{2}m_1 n_1 (u_2-u_1)\Big[\gamma(u_2-u_1)^2 + 5\gamma\left(\frac{k}{m_2}\right)(T_2-T_1) + \frac{5k}{2m}\left(\frac{m_1+m_2}{m_2}\right)^2 T_1\Big]\Big\} , \tag{15}$$

$$\frac{dq_2}{dt} = \frac{1}{4}\nu_{22}(\gamma-3)q_2 + 2\nu_{21}\left(\frac{m_1}{m_1+m_2}\right)^3\Big\{\frac{m_2}{m_1}\frac{n_2}{n_1}q_1 - \Big[\gamma-(1+\gamma)\left(\frac{m_1+m_2}{m_1}\right)$$

$$+\frac{3}{2}\left(\frac{m_1+m_2}{m_1}\right)^2\Big]q_2 - \gamma\frac{m_2}{m_1}\frac{n_2}{n_1}(u_2-u_1)P_1 - (u_2-u_1)P_2\Big[\gamma-\left(\frac{1}{4}\gamma+\frac{3}{2}\right)\left(\frac{m_1+m_2}{m_1}\right)$$

$$+\frac{1}{2}\left(\frac{m_1+m_2}{m_1}\right)^2\Big] - \frac{1}{2}m_2 n_2 (u_2-u_1)\Big[\gamma(u_2-u_1)^2 + 5\frac{\gamma k}{m_1}(T_1-T_2)$$

$$+5\frac{k}{m_2}\left(\frac{m_1+m_2}{m_1}\right)^2 T_2\Big]\Big\} . \tag{16}$$

To obtain these equations in dimensionless form a simple change of variable is necessary. If $t = 0$, then $u_1 = u_{10}$, $u_2 = u_{20}$, $T_1 = T_{10}$, $T_2 = T_{20}$, $P_1 = P_{10}$, $P_2 = P_{20}$, $q_1 = q_{10}$, $q_2 = q_{20}$. So, let $u_1' = u_1/u_{10}$, $u_2' = u_2/u_{20}$, $T_1' = T_1/T_{10}$, $T_2' = T_2/T_{20}$, $P_1' = P_1/P_{10}$, $P_2' = P_2/P_{20}$, $q_1' = q_1/q_{10}$, $q_2' = q_2/q_{20}$, and $z_{11} = t\nu_{11}$. We now take the derivative with respect to a collision number instead of time. Using Walker and Tanenbaum's expression for the cross-collision frequency, the respective cross-collision frequency ratios are determined for these equations assuming that the interparticle force constant ratios are all equal to unity. These frequency ratios are:

$$\frac{\nu_{12}}{\nu_{11}} = \left[\frac{m_1 + m_2}{2m_2}\right]^{\frac{1}{2}} \frac{n_2}{n_1} \quad ;$$

$$\frac{\nu_{21}}{\nu_{11}} = \left[\frac{m_1 + m_2}{2m_2}\right]^{\frac{1}{2}} \quad ;$$

and

$$\frac{\nu_{22}}{\nu_{11}} = \left[\frac{m_1}{m_2}\right]^{\frac{1}{2}} \frac{n_2}{n_1} \quad .$$

Substituting these variable changes and cross-collision frequency ratios into equations (9) - (16), rearranging terms, and letting $m = m_1/m_2$, $n = n_1/n_2$, $u = u_{10}/u_{20}$, $P = P_{10}/P_{20}$, $T = T_{10}/T_{20}$, $q = q_{10}/q_{20}$, $K_1 = \frac{1}{2}m_1 u_{10}^2$, $K_2 = \frac{1}{2}m_2 u_{20}^2$, $E_1 = 3/2kT_{10}$, $E_2 = 3/2kT_{20}$, $P_{R1} = n_1 m_1 u_{10}^2/P_{10}$, $P_{R2} = n_2 m_2 u_{20}^2/P_{20}$, $Q_{R1} = \frac{1}{2}u_{10} m_1 n_1 u_{10}^2/q_{10}$, and $Q_{R2} = \frac{1}{2}u_{20} m_2 n_2 u_{20}^2/q_{20}$, the following equations are obtained:

momentum,

$$\frac{du_1'}{dz_{11}} = \left[\frac{1}{2}(m+1)\right]^{\frac{1}{2}} \frac{1}{n(m+1)} \left(\frac{u_2'}{u} - u_1'\right) \quad , \tag{17}$$

$$\frac{du_2'}{dz_{11}} = -\left[\frac{1}{2}(m+1)\right]^{\frac{1}{2}} \frac{m}{m+1} \left(u_2' - u u_1'\right) \quad ; \tag{18}$$

translational energy,

$$\frac{dT_1'}{dz_{11}} = \frac{4}{3n}\left[\frac{1}{2}(m+1)\right]^{\frac{1}{2}} \frac{1}{(m+1)^2}\left[\frac{3}{2} m\left(\frac{T_2'}{T} - T_1'\right) + \frac{3}{2}\frac{K_1}{E_1}\left(\frac{u_2'}{u} - u_1'\right)^2\right] , \tag{19}$$

$$\frac{dT_2'}{dz_{11}} = \frac{4}{3}\left[\frac{1}{2}(m+1)\right]^{\frac{1}{2}}\left[\frac{m}{(m+1)}\right]^2\left[-\frac{3}{2}\,\frac{1}{m}\left(T_2'-TT_1'\right)+\frac{3}{2}\,\frac{K_2}{E_2}\left(u_2'-uu_1'\right)^2\right]; \quad (20)$$

viscous stress,

$$\frac{dP_1'}{dz_{11}} = (\beta-1)P_1' + \frac{2\beta}{n}\left[\frac{1}{2}(m+1)\right]^{\frac{1}{2}}\left(\frac{1}{m+1}\right)^2\left\{\left[1-\frac{1}{\beta}(m+1)\right]P_1' + \frac{P_{R1}}{u^2 P_{R2}}P_2'\right.$$

$$\left. + \frac{3}{2}P_{R1}\left(\frac{u_2'}{u}-u_1'\right)^2\right\}, \quad (21)$$

$$\frac{dP_2'}{dz_{11}} = (\beta-1)\frac{m_2}{n}P_2' + 2\beta\left[\frac{1}{2}(m+1)\right]^{\frac{1}{2}}\left(\frac{m}{m+1}\right)^2\left[\left(1-\frac{1}{\beta}\,\frac{m+1}{m}\right)P_2' + \frac{u^2 P_{R2}}{P_{R1}}P_1'\right.$$

$$\left. + \frac{2}{3}P_{R2}\left(u_2'-uu_1'\right)^2\right]; \quad (22)$$

translational heat flux,

$$\frac{dq_{t1}'}{dz_{11}} = \frac{1}{4}(\gamma-3)q_{t1}' + \frac{2}{n}\left[\frac{1}{2}(m+1)\right]^{\frac{1}{2}}\left(\frac{1}{m+1}\right)^3\left\{\frac{mn}{q}q_{t2}' - \left[\gamma-(1+\gamma)(m+1)\right.\right.$$

$$\left. + \frac{3}{2}(m+1)^2\right]q_{t1}' + 2\frac{\gamma Q_{R1}}{u^2 P_{R2}}\left(\frac{u_2'}{u}-u_1'\right)P_2' + \frac{2Q_{R1}}{P_{R1}}\left(\frac{u_2'}{u}-u_1'\right)\left[\gamma\right.$$

$$\left. -\left(\frac{1}{4}\gamma+\frac{3}{2}\right)(m+1) + \frac{1}{2}(m+1)^2\right]P_1' + Q_{R1}\left(\frac{u_2'}{u}-u_1'\right)\left[\gamma\left(\frac{u_2'}{u}-u_1'\right)^2\right.$$

$$\left.\left. + \frac{5\gamma}{3}\,\frac{E_1 m}{K_1}\left(\frac{T_2'}{T}-T_1'\right) + \frac{5}{6}\,\frac{E_1}{K_1}(m+1)^2 T_1'\right]\right\}, \quad (23)$$

$$\frac{dq_{t2}'}{dz_{11}} = \frac{m^{\frac{1}{2}}}{4n}(\gamma-3)q_{t2}' + 2\left[\frac{1}{2}(m+1)\right]^{\frac{1}{2}}\left(\frac{m}{m+1}\right)^3\left\{\frac{q}{mn}q_{t1}' - \left[\gamma-(1+\gamma)\left(\frac{m+1}{m}\right)\right.\right.$$

$$\left. + \frac{3}{2}\left(\frac{m+1}{m}\right)^2\right]q_{t2}' - \frac{2\gamma Q_{R2}u^2}{P_{R1}}\left(u_2'-uu_1'\right)P_1'$$

$$- \frac{2Q_{R2}}{P_{R2}}\left(u_2'-uu_1'\right)\left[\gamma-\left(\frac{1}{4}\gamma+\frac{3}{2}\right)\left(\frac{m+1}{m}\right)+\frac{1}{2}\left(\frac{m+1}{m}\right)^2\right]P_2'$$

$$\left. - Q_{R2}\left(u_2'-uu_1'\right)\left[\gamma\left(u_2'-uu_1'\right)^2 + \frac{5\gamma}{3}\left(TT_1'-T_2'\right) + \frac{5}{6}\,\frac{E_2}{K_2}\left(\frac{m+1}{m}\right)^2 T_2'\right]\right\}. \quad (24)$$

These resulting equations form a set of dimensionless coupled differential equations, the analytical solution of which is quite involved. Upon examination, however, it would be relatively simple to solve equations (17) - (20) analytically. These equations may first be simplified by defining some new constants as $A = m + 1$, $B = \left[\frac{1}{2}(m + 1)\right]^{\frac{1}{2}}$, $L = E_1/K_1$, and $W = E_2/K_2$. Substituting these definitions into equations (17) - (20) and rearranging yields:

$$\frac{du_1'}{dz_{11}} = \frac{B}{An}\left(\frac{u_2'}{u} - u_1'\right) \quad ; \tag{25}$$

$$\frac{du_2'}{dz_{11}} = -\frac{Bm}{A}\left(u_2' - uu_1'\right) ; \tag{26}$$

$$\frac{dT_1'}{dz_{11}} = \frac{2Bm}{nA^2}\left(\frac{T_2'}{T} - T_1'\right) + \frac{2B}{nA^2L}\left(\frac{u_2'}{u} - u_1'\right)^2 ; \tag{27}$$

$$\frac{dT_2'}{dz_{11}} = \frac{-2Bm}{nA^2}\left(T_2' - TT_1'\right) + \frac{2Bm^2}{A^2W}\left(u_2' - uu_1'\right)^2 . \tag{28}$$

The following method may be used to solve equations (25) and (28) for $\frac{u_2'}{u} - u_1'$. Dividing equation (26) by u, subtracting equation (25) from the result, and rearranging yields

$$\frac{d\left(\frac{u_2'}{u} - u_1'\right)}{\left(\frac{u_2'}{u} - u_1'\right)} = -\frac{B}{A}\left(m + \frac{1}{n}\right) dz_{11} \quad ,$$

the solution of which is

$$\frac{u_2'}{u} - u_1' = (\text{constant})\, e^{\left[-\frac{B}{A}\left(m + \frac{1}{n}\right) z_{11}\right]} .$$

At $z_{11} = 0$, then $u_1' = u_2' = 1$, and the constant of integration is $\frac{1 - u}{u}$. Therefore, the complete solution is

$$\frac{u_2'}{u} - u_1' = \left(\frac{1-u}{u}\right) e^{\left[-\frac{B}{A}\left(m + \frac{1}{n}\right) z_{11}\right]} . \tag{29}$$

For simplicity, let $A_1 = \frac{B}{A}\left(m + \frac{1}{n}\right)$ and $C = \frac{u_2'}{u} - u_1'$. This substitution into equation (29) gives the solution as

$$C = \left(\frac{1-u}{u}\right) e^{-A_1 z_{11}}. \tag{30}$$

The same method may be used to solve equations (27) and (28) for $\frac{T_2'}{T} - T_1'$. Dividing equation (28) by T, subtracting equation (27) from the result, and rearranging yields

$$\frac{d}{dz_{11}}\left(\frac{T_2'}{T} - T_1'\right) = \frac{-2Bm}{A^2}\left(1+\frac{1}{n}\right)\left(\frac{T_2'}{T} - T_1'\right) + \frac{2B}{A^2}\left(\frac{m^2u^2}{W} - \frac{1}{nL}\right)\left(\frac{u_2'}{u} - u_1'\right). \tag{31}$$

For simplicity, let $F = \frac{T_2'}{T} - T_1'$, $A_2 = \frac{2Bm}{A^2}(1 + \frac{1}{n})$, $B_1 = \frac{2B}{A^2}(\frac{m^2u^2}{W} - \frac{1}{nL})$, and $B_2 = B_1(\frac{1-u}{u})^2$. Substituting these into equation (31) gives

$$\frac{dF}{dz_{11}} + A_2 F = B_2 e^{-2A_1 z_{11}}.$$

This is a differential equation of the form:

$$\frac{dy}{dx} + P(x) = Q(x),$$

which has a solution of the form

$$Y = e^{-\int P(x)dx}\left[\int Q(x) e^{\int P(x)dx} dx + \text{constant}\right].$$

Therefore, the solution for F is

$$F = e^{-A_2 z_{11}}\left[\frac{B_2}{A_2 - 2A_1} e^{(A_2 - 2A_1)z_{11}} + C_2\right],$$

or

$$F = \frac{B_2}{A_2 - 2A_1} e^{-2A_1 z_{11}} + C_2 e^{-A_2 z_{11}}, \tag{32}$$

where C_2 is the constant of integration. If $z_{11} = 0$, then $F = \frac{1}{T} - 1$, and the constant of integration is $C_2 = \frac{1-T}{T} - \frac{B_2}{A_2 - 2A_1}$. For simplicity, let $C_1 = \frac{B_2}{A_2 - 2A_1}$ and $C_2 = \frac{1-T}{T} - C_1$. Substituting this into equation (32) gives

$$F = C_1 e^{-2A_1 z_{11}} + C_2 e^{-A_2 z_{11}} . \tag{33}$$

Now, it is desirable to solve for T_1' and T_2' since these quantities appear alone in equations (23) and (24). Substituting equations(30) and (33) into equation (27) and rearranging gives

$$\frac{dT_1'}{dz_{11}} = \frac{2B}{nA^2}\left[mC_1 e^{-2A_1 z_{11}} + mC_2 e^{-A_2 z_{11}} + \frac{1}{L}\left(\frac{1-u}{u}\right)^2 e^{-2A_1 z_{11}}\right].$$

The solution for T_1' may be found simply by integrating to yield, after rearranging,

$$T_1' = \frac{-2B}{nA^2}\left\{\frac{1}{2A_1}\left[mC_1 + \frac{1}{L}\left(\frac{1-u}{u}\right)^2\right] e^{-2A_1 z_{11}} + \frac{mC_2}{A_2} e^{-A_2 z_{11}}\right\} + C_5 ,$$

where C_5 is the constant of integration. If $z_{11} = 0$, then $T_1' = 1$, thus giving

$$C_5 = 1 + \frac{2B}{nA^2}\left[\frac{1}{2A_1}\left(mC_1 + \frac{1}{L}\left(\frac{1-u}{u}\right)^2\right] + \frac{mC_2}{A_2} .$$

For simplicity, let

$$C_3 = \frac{2B}{2nA^2A_1}\left[mC_1 + \frac{1}{L}\left(\frac{1-u}{u}\right)^2\right] \text{ and } C_4 = \frac{2BmC_2}{nA^2A_2} ,$$

so that $C_5 = 1 + C_3 + C_4$. The result is that

$$T_1' = -C_3 e^{-2A_1 z_{11}} - C_4 e^{-A_2 z_{11}} + C_5 .$$

From the definition of $F = \frac{T_2'}{T} - T_1'$, we can solve for T_2' since we now know T_1', obtaining

$$T_2' = T(F + T_1') .$$

In summary, then, the equations to be solved numerically are equations (17) - (22) where,

$$T_1' = -C_3 e^{-2A_1 z_{11}} - C_4 e^{-A_2 z_{11}} + C_5 \;;$$

$$T_2' = T(F + T_1');$$

$$\frac{T_2'}{T} - T_1' = F = C_1 e^{-2A_2 z_{11}} + C_2 e^{-A_2 z_{11}} \;;$$

$$\frac{u_2'}{u} - u_1' = C = \left(\frac{1-u}{u}\right) e^{-A_1 z_{11}} \;.$$

III. PROGRAMMING CONSIDERATIONS

The dimensionless differential equations were solved numerically using the IBM 360/75 located at Triangle Universities Computation Center. The program for the solution consists of four main parts:

a. A driving program.

b. A subroutine HPCG, available in the IBM Scientific Subroutine Package, for solving a set of first order ordinary differential equations.

c. A subroutine FCT required by HPCG which defines the differential equations to be solved.

d. A subroutine OUTP required by HPCG which regulates the output of the program.

A listing of the program is given in the appendix. In order to define the differential equations for the program in the subroutine FCT and to print out the required information in the subroutine OUTP, it was necessary to rename the variables and constants used previously. This renaming was quite extensive. To aid with the transition from the theoretical equations to the programmed equations, the renaming procedure is summarized in Table I. As an aid to the reader, a listing of the expressions used in the program to simplify calculations is given in Table II.

The solution technique utilized by the subroutine HPCG is an integration method known as Hamming's modified predictor-corrector method. It obtains an approximate solution of a general system of first-order ordinary differential equations with given initial values. (For a detailed description of the procedure, one should refer to reference 3.) The initial values for the dependent and independent variables, the beginning and end points of the integration range, the initial integration increment, and various error parameters are obtained and saved by the main program. The required data for the subroutines FCT and OUTP are the values for n, m, P, q, and T and are read in at appropriate places in the subroutines.

Two versions of the OUTP subroutine serving two different purposes by the user are given in the program listing. The general purpose of both versions are naturally to generate a printing of the information required from the program. Version I simply generates a solution to the dimensionless equations for two colliding gases. Version II creates an entirely different form of output. In essence, it prints relaxation collision numbers for each of the computed dimensionless variables of "temperature difference", TEM = $(T_2'/T - T_1')$, "stresses", P_1' and P_2', and "heat fluxes", q_1' and q_2' for two gases going in the same direction.** Version II accomplishes that end in the following manner. By using a series of If-statements, the subroutine checks each value of P_1', P_2', q_1', and q_2' to see if it has reached 1/e of its initial value. If that value has been reached, the value of the corresponding z_{11} value is printed. When this condition for all four of the variables is satisfied, the subroutine

---

**The quotations emphasize that the obtained information is actually in dimensionless form.

continues to increment z_{11} and calculate the temperature difference of $T_2'/T - T_1'$ until that quantity has reached 1/e of its initial value. When that value has been reached, the corresponding z_{11} is printed. At this point, the ratios of the respective z_{11}'s to the z_{11} for the temperature difference is calculated and printed. Also printed for each value of z_{11} are the values of the velocity and temperature differeneces, VEL and TEM respectively, P_1', P_2', q_1', q_2', and cross-collision frequencies z_{12}, z_{21}, and z_{22}. Now, the values for the dependent and independent variables are re-initialized, a new set of data is read by the subroutines, and the procedure is restarted.

TABLE I

Renaming of the Variables and Constants for Use in the Program

Theoretical Equations	Program
z_{11}	X
T_1'	Y3
T_2'	Y4
P_1'	Y(1)
P_2'	Y(2)
q_1'	Y(3)
q_2'	Y(4)
$u_2'/u - u_1'$	C
$u_2' - uu_1'$	D
$T_2'/T - T_1'$	F
$T_2' - TT_1'$	G
dP_1'/dz_{11}	DERY(1)
dP_2'/dz_{11}	DERY(2)
dq_1'/dz_{11}	DERY(3)
dq_2'/dz_{11}	DERY(4)
m	M
n	N
u	U
T	T
P	P

Theoretical Equations	Program
q	Q
E_1/K_1	L
E_2/K_2	W
$n_1m_1u_{10}{}^2/P_{10}$	PR1
$n_2m_2u_{20}{}^2/P_{20}$	PR2
$\frac{1}{2}u_{10}n_1m_1u_{10}{}^2/q_{10}$	QR1
$\frac{1}{2}u_{20}n_2m_2u_{20}{}^2/q_{20}$	QR2
$m + 1$	A
$\left[\frac{1}{2}(m + 1)\right]^{\frac{1}{2}}$	B
$\left[\frac{(1 - u)}{u}\right]^2$	ART
A_1	A1
A_2	A2
B_1	B1
B_2	B2
$C_1 - C_8$	C1 - C8

TABLE II

Expressions Used in the Program to Simplify Calculations

Expression Name	Expression
H	$PR1/u^2 PR2$
I	$QR1/u^2 PR2$
J	QR1/PR1
Z	QR2/PR1
ZZ	QR2/PR2
E	B/N

IV. SUMMARY AND CONCLUSIONS

The aforementioned equations were solved numerically by the computer program listed in the Appendix. The values of the program parameters PR1 = 3.0×10^{24} and QR1 = 1.0×10^{24} were chosen for the colliding gas case and the values PR1 = 30 and QR1 = 10 were used for the case of the two gases traveling in the same direction. These values were chosen to satisfy an assumption used in deriving the 13-Moment equations, viz., that the stresses and heat fluxes represent small departures from equilibrium.[1]

The solutions are plotted as shown in Figs. 1 - 5. In the case of the colliding gases, the heat fluxes and stresses are initially zero but grow with the increase in the collision number, z_{11}. This occurence is a consequence of the mathematics in that the heat flux and stress equations have terms containing velocity and temperature differences which are not always zero. For reference sake, we call the portion of the gaseous mixture containing type 1 molecules, gas 1, and that containing type 2 molecules, gas 2. In the case of equal densities and masses and initially equal temperatures (Fig. 1), the dimensionless variables behave the same for both gases. The temperature difference remains zero and the velocity difference is a decaying exponential. As the velocity difference decreases, the temperature of both gases increases indicating a transfer of energy from localized translational energy to random thermal energy. As the mass of the molecules in gas 2 is increased, holding the density of both gases the same, there is a marked seperation of the dimensionless variable curves (Fig. 2). The heat flux and stress curves increase to a maximum and then begin to decrease to zero. This decrease for both curves for the lighter gas begins at a smaller collision number. Also, the lighter gas approaches a constant temperature long before the heavier gas. As in Fig. 1, while the velocity difference decreases, the temperature of both gases increases, the lighter gas increasing much faster than the heavier gas. In Fig. 3, where the mass of the molecules in gas 2 is further increased, the same type of results are obtained. These occurences are qualitatively predicted by Morse.[2] He says that in a gaseous mixture, the lighter species will equilibrate before the heavier species.

The case for various mass ratios having a density ratio of 0.1 was also computed for these colliding gases. The graphs are not included here, but they are the same as for equal density ratios. The only difference is that the curves peak much more sharply than in the equal density case.

In Figs. 4 and 5, the ratios of the respective relaxation collision numbers to the relaxation collision number for the temperature difference is plotted as a function of the mass ratios. In both figures, the curves have generally the same shape. Changing the density ratio from n = 1.0 to n = 0.5, lowers the curves by a small amount with the exception of the q_2' curve which is raised for a mass ratio larger than about 0.10. It should be also noted from these graphs that for mass ratios equal to and below 0.01, the values of the relaxation collision numbers q_2' and P_2' compared to the relaxation collision number for the temperature difference is not negligible, ranging from 0.15 to 0.38 for q_2' and from 0.11 to 0.30 for P_2', for a density ratio of n = 1.0. This means that extreme caution must be used when saying that the heat flux and stress for the heavier gas relax much faster than the temperature difference between the two components of the mixture.

Fig. 1. Plot of dimensionless variables as a function of collision number, z_{11}, for n = 1 and m = 1

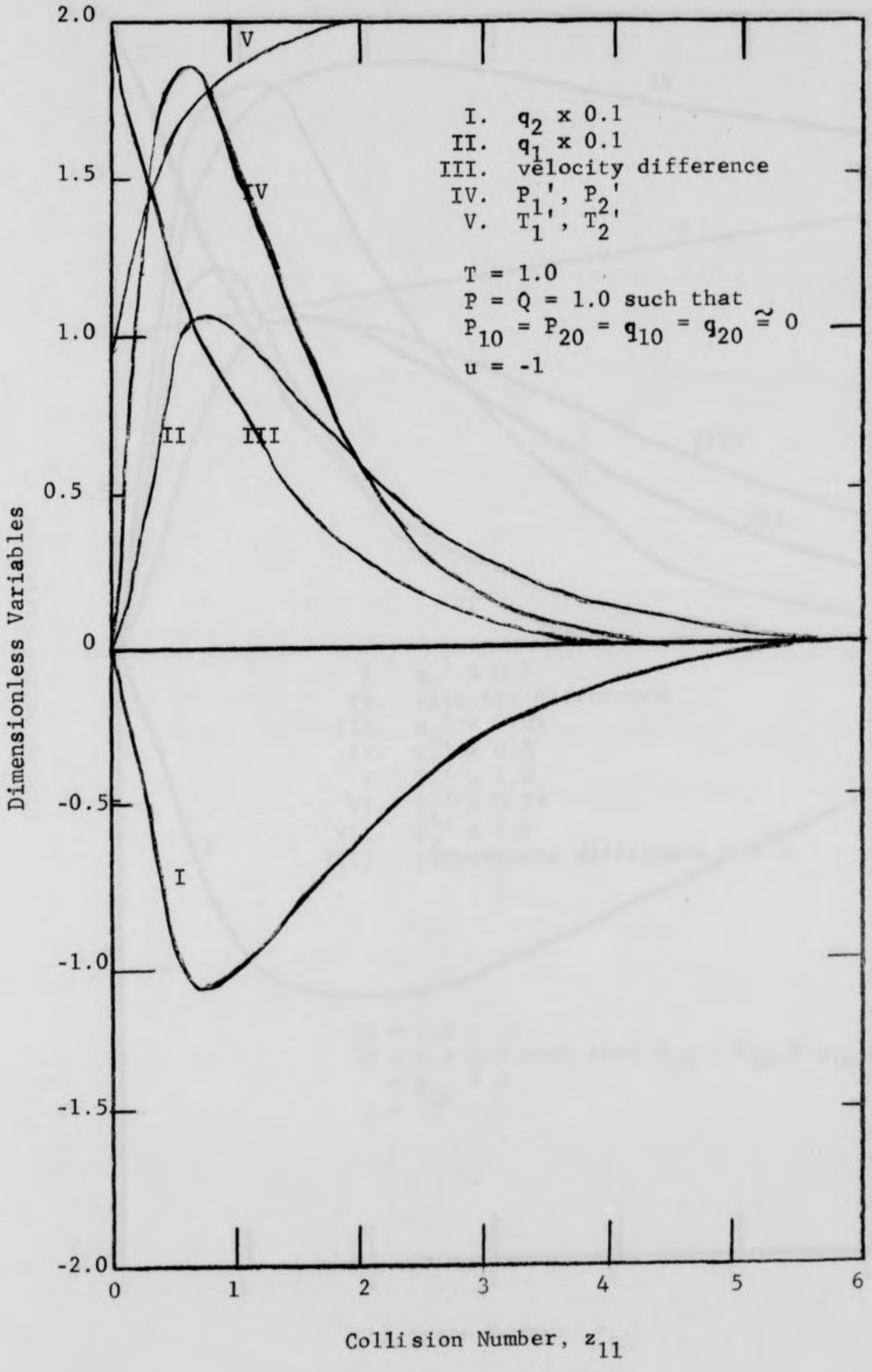


Fig. 2. Plot of dimensionless variables as a function of collision number, z_{11}, for n = 1 and m = 0.1

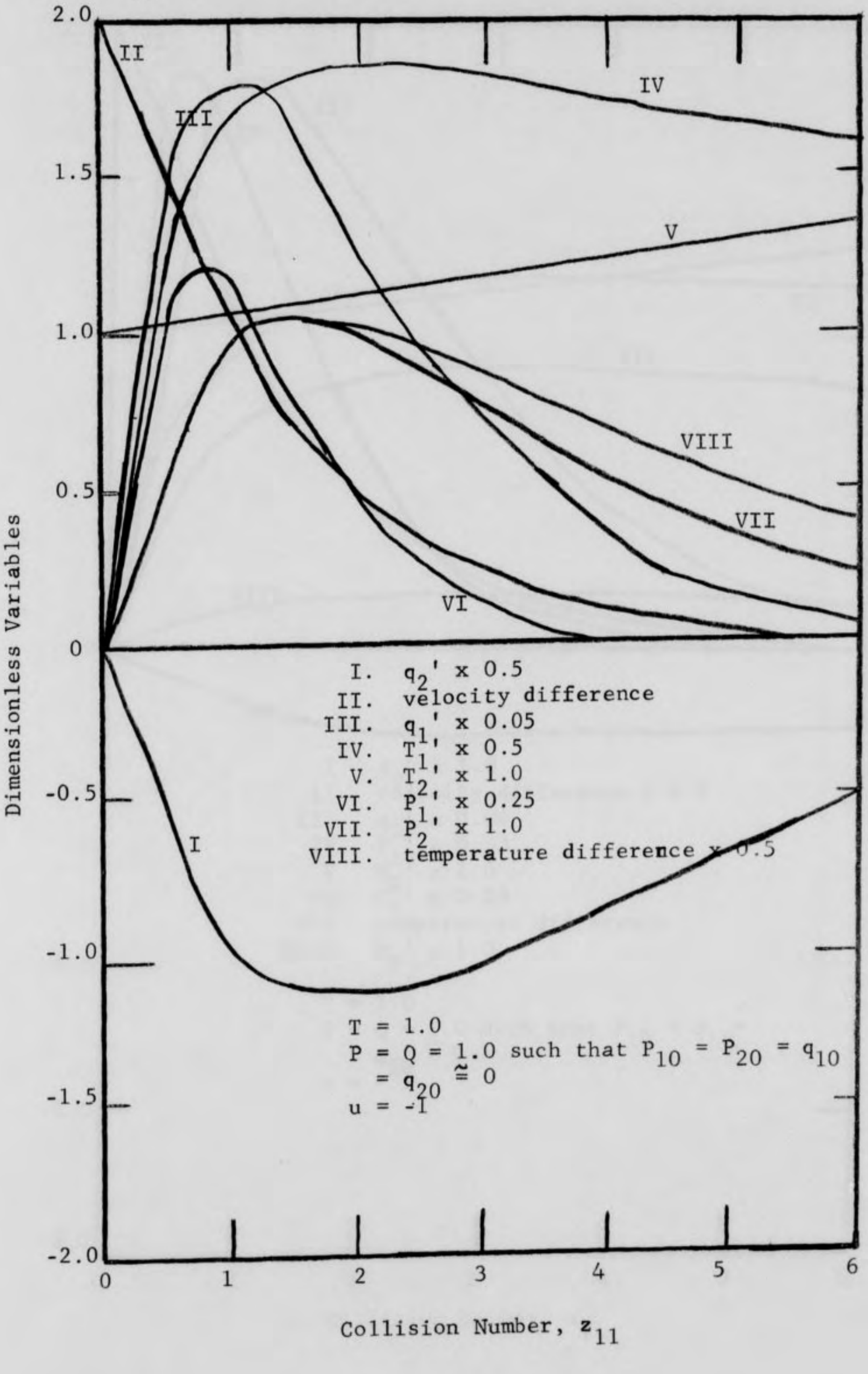


Fig. 3. Plot of dimensionless variables as a function of collision number, z_{11}, for n = 1 and m = 0.01

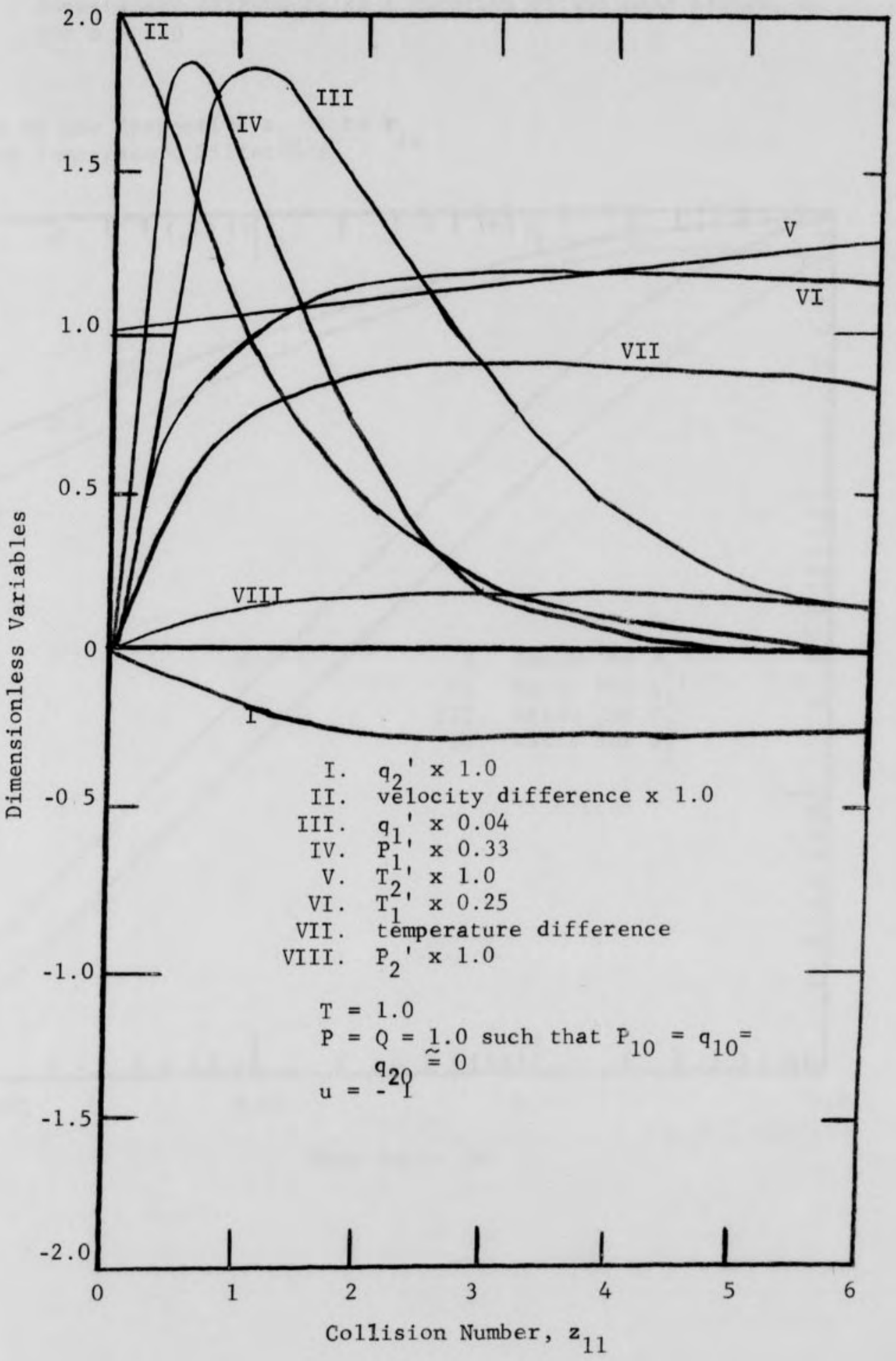
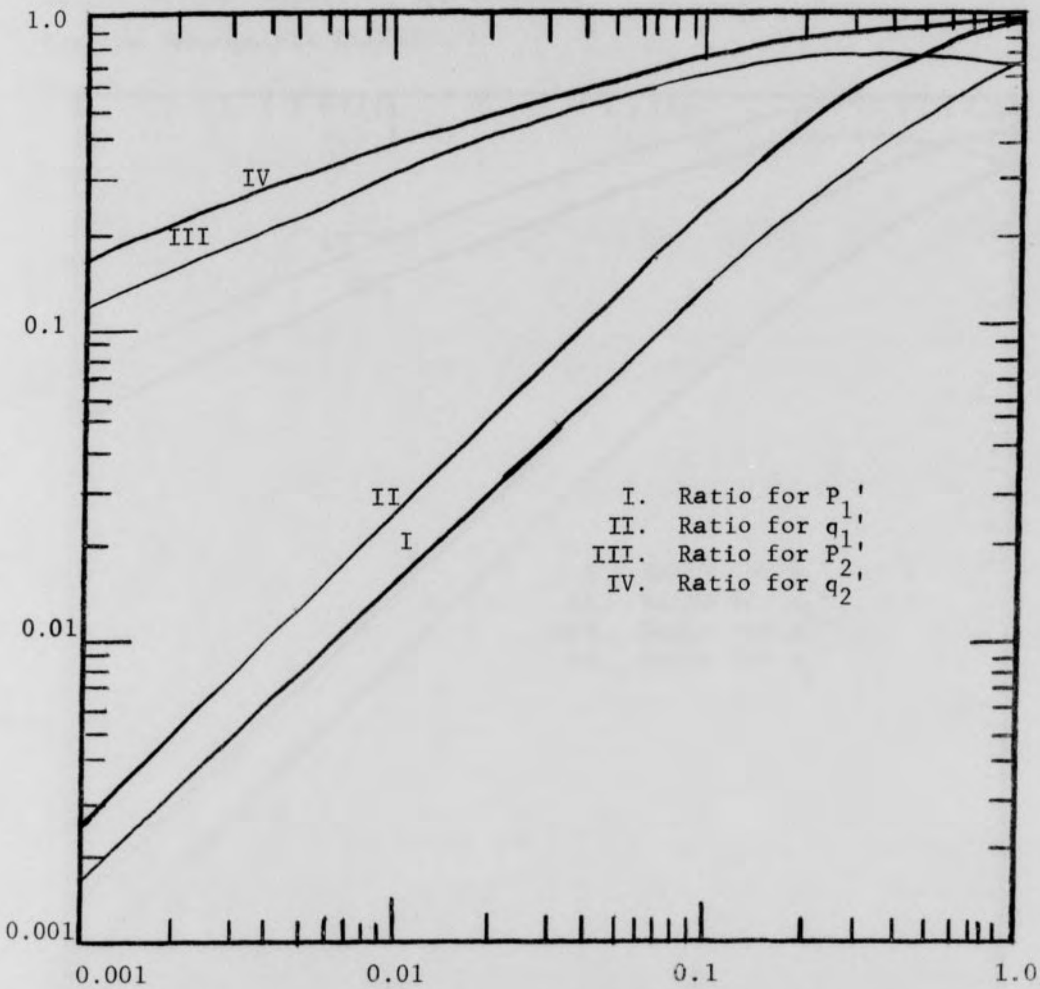


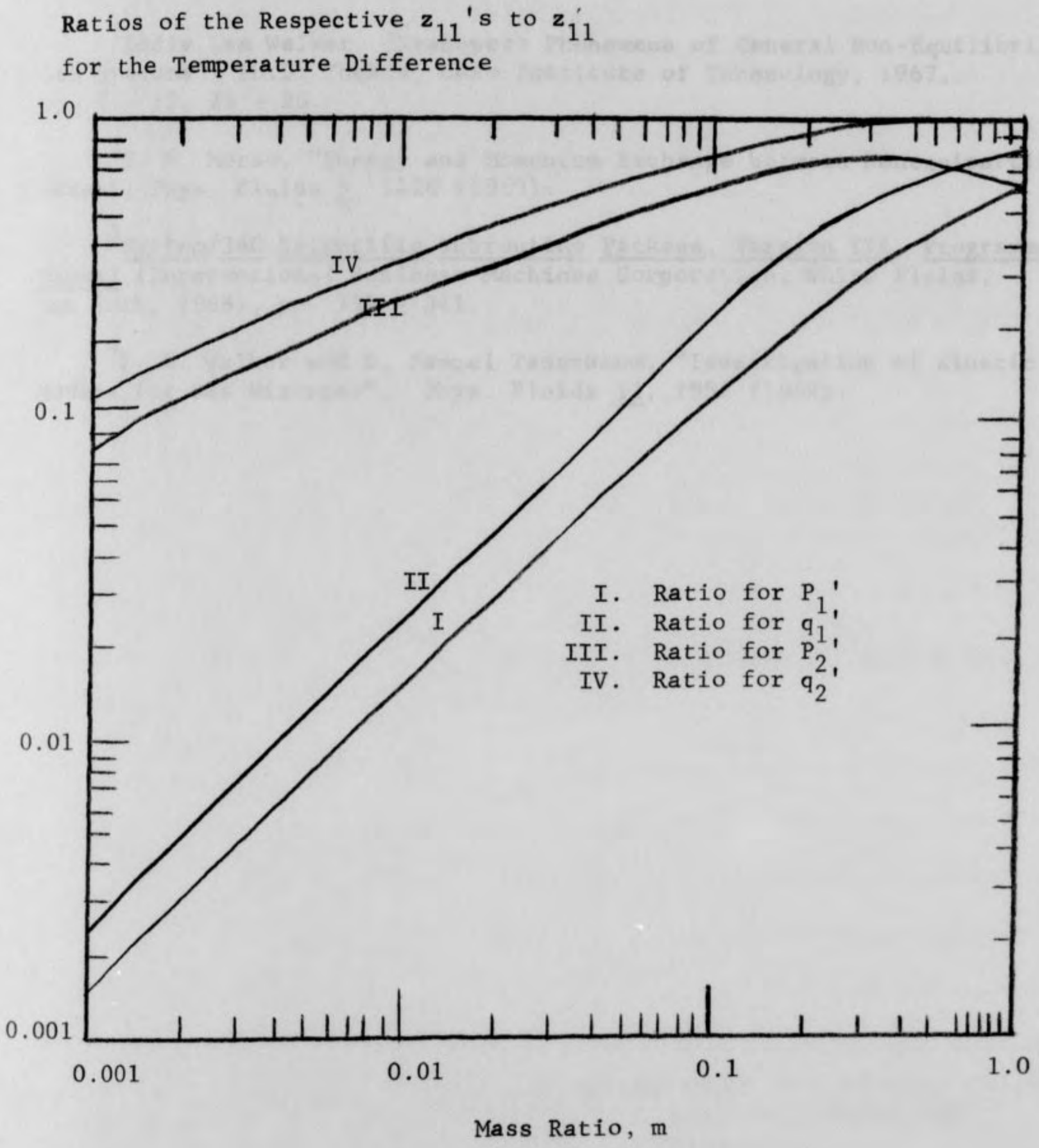
Fig. 4. Plot of the ratios of the respective z_{11}'s to z_{11} for the temperature difference as a function of the mass ratios, m, for n = 1.0

Ratios of the Respective z_{11}'s to z_{11} for the Temperature Difference



Mass Ratio, m

Fig. 5. Plot of the ratios of the respective z_{11}'s to z_{11} for the temperature difference as a function of the mass ratios, m, for n = 0.5



REFERENCES

[1] Eddie Lee Walker, "Transport Phenomena of General Non-Equilibrium Gas Systems", Ph.D. Thesis, Case Institute of Technology, 1967, pp. 7 - 12, 23 - 26.

[2] T. F. Morse, "Energy and Momentum Exchange between Nonequipartition Gases", Phys. Fluids _6_, 1420 (1963).

[3] _System/360 Scientific Subroutine Package, Version III, Programmer's Manual_ (International Business Machines Corporation, White Plains, New York, 1968), pp. 337 - 341.

[4] E. L. Walker and B. Samuel Tanenbaum, "Investigation of Kinetic Models for Gas Mixtures", Phys. Fluids _11_, 1951 (1968).

APPENDIX

PROGRAM LISTING

```
C THE FOLLOWING IS THE MAIN PROGRAM.
      REAL M,N,K1,K2,I,L,J
      DIMENSION Y(4),DERY(4),PRMT(5),AUX(16,4),SA(2)
      DIMENSION SERY(4),SY(4),SRMT(4)
      EXTERNAL FCT,OUTP
  102 READ,NDIM
C THE INITIAL   VALUES OF THE DEPENDENT VARIABLES AND THEIR DERIVATIVES,
C THE INITIAL AND FINAL VALUES OF THE INDEPENDENT VARIABLE, THE INCREMENT
C OF THE INDEPENDENT VARIABLE, AND VARIOUS ERROR PARAMETERS ARE READ
C IN AND STORED HERE.
      READ,(DERY(JJ),JJ=1,NDIM)
      READ,(Y(JJ),JJ=1,NDIM)
      READ,(PRMT(JJ),JJ=1,4)
      SDIM=NDIM
      DO 7 II=1,NDIM
      SERY(II)=DERY(II)
    7 SY(II)=Y(II)
      DO 8 II=1,4
    8 SRMT(II)=PRMT(II)
    9 CALL HPCG(PRMT,Y,DERY,NDIM,IHLF,FCT,OUTP,AUX)
C NOMO IS A SEGMENT OF DATA INDICATING WHETHER OR NOT A NEW SET OF
C DATA IS TO BE READ INTO THE PROGRAM.
      READ,NOMO
      IF(NOMO)102,101,100
  100 NDIM=SDIM
      DO 71 II=1,NDIM
      DERY(II)=SERY(II)
   71 Y(II)=SY(II)
      DO 81 II=1,4
   81 PRMT(II)=SRMT(II)
      GO TO 9
  101 STOP
      END

C THE FOLLOWING IS THE SUBROUTINE WHICH DOES THE ACTUAL INTEGRATION.
      SUBROUTINE HPCG(PRMT,Y,DERY,NDIM,IHLF,FCT,OUTP,AUX)                HP
      DIMENSION PRMT(5),Y(4),DERY(4),AUX(16,4)
      N=1                                                                HP
      IHLF=0                                                             HP
      X=PRMT(1)                                                          HP
```

```
      H=PRMT(3)
      PRMT(5)=0.
      DO 1 I=1,NDIM
      AUX(16,I)=0.
      AUX(15,I)=DERY(I)
    1 AUX(1,I)=Y(I)
      IF(H*(PRMT(2)-X))3,2,4
    2 IHLF=12
      GOTO 4
    3 IHLF=13
    4 CALL FCT(X,Y,DERY)
      CALL OUTP(X,Y,DERY,IHLF,NDIM,PRMT)
      IF(PRMT(5))6,5,6
    5 IF(IHLF)7,7,6
    6 RETURN
    7 DO 8 I=1,NDIM
    8 AUX(8,I)=DERY(I)
      ISW=1
      GOTO 100
    9 X=X+H
      DO 10 I=1,NDIM
   10 AUX(2,I)=Y(I)
   11 IHLF=IHLF+1
      X=X-H
      DO 12 I=1,NDIM
   12 AUX(4,I)=AUX(2,I)
      H=.5*H
      N=1
      ISW=2
      GOTO 100
   13 X=X+H
      CALL FCT(X,Y,DERY)
      N=2
      DO 14 I=1,NDIM
      AUX(2,I)=Y(I)
   14 AUX(9,I)=DERY(I)
      ISW=3
      GOTO 100
   15 DELT=0.
      DO 16 I=1,NDIM
   16 DELT=DELT+AUX(15,I)*ABS(Y(I)-AUX(4,I))
      DELT=.06666667*DELT
      IF(DELT-PRMT(4))19,19,17
   17 IF(IHLF-10)11,18,18
   18 IHLF=11
      X=X+H
      GOTO 4
   19 X=X+H
      CALL FCT(X,Y,DERY)
      DO 20 I=1,NDIM
      AUX(3,I)=Y(I)
```

```
   20 AUX(10,I)=DERY(I)
      N=3
      ISW=4
      GOTO 100
   21 N=1
      X=X+H
      CALL FCT(X,Y,DERY)
      X=PRMT(1)
      DO 22 I=1,NDIM
      AUX(11,I)=DERY(I)
   22 Y(I)=AUX(1,I)+H*(.375*AUX(8,I)+.7916667*AUX(9,I)
     1-.2083333*AUX(10,I)+.04166667*DERY(I))
   23 X=X+H
      N=N+1
      CALL FCT(X,Y,DERY)
      CALL OUTP(X,Y,DERY,IHLF,NDIM,PRMT)
      IF(PRMT(5))6,24,6
   24 IF(N-4)25,200,200
   25 DO 26 I=1,NDIM
      AUX(N,I)=Y(I)
   26 AUX(N+7,I)=DERY(I)
      IF(N-3)27,29,200
   27 DO 28 I=1,NDIM
      DELT=AUX(9,I)+AUX(9,I)
      DELT=DELT+DELT
   28 Y(I)=AUX(1,I)+.3333333*H*(AUX(8,I)+DELT+AUX(10,I))
      GOTO 23
   29 DO 30 I=1,NDIM
      DELT=AUX(9,I)+AUX(10,I)
      DELT=DELT+DELT+DELT
   30 Y(I)=AUX(1,I)+.375*H*(AUX(8,I)+DELT+AUX(11,I))
      GOTO 23
  100 DO 101 I=1,NDIM
      Z=H*AUX(N+7,I)
      AUX(5,I)=Z
  101 Y(I)=AUX(N,I)+.4*Z
      Z=X+.4*H
      CALL FCT(Z,Y,DERY)
      DO 102 I=1,NDIM
      Z=H*DERY(I)
      AUX(6,I)=Z
  102 Y(I)=AUX(N,I)+.2969776*AUX(5,I)+.1587596*Z
      Z=X+.4557372*H
      CALL FCT(Z,Y,DERY)
      DO 103 I=1,NDIM
      Z=H*DERY(I)
      AUX(7,I)=Z
  103 Y(I)=AUX(N,I)+.2181004*AUX(5,I)-3.050965*AUX(6,I)+3.832865*Z
      Z=X+H
      CALL FCT(Z,Y,DERY)
      DO 104 I=1,NDIM
```

```
1040Y(I)=AUX(N,I)+.1747603*AUX(5,I)-.5514807*AUX(6,I)
   1+1.205536*AUX(7,I)+.1711848*H*DERY(I)
    GOTO(9,13,15,21),ISW
200 ISTEP=3
201 IF(N-8)204,202,204
202 DO 203 N=2,7
    DO 203 I=1,NDIM
    AUX(N-1,I)=AUX(N,I)
203 AUX(N+6,I)=AUX(N+7,I)
    N=7
204 N=N+1
    DO 205 I=1,NDIM
    AUX(N-1,I)=Y(I)
205 AUX(N+6,I)=DERY(I)
    X=X+H
206 ISTEP=ISTEP+1
    DO 207 I=1,NDIM
   0DELT=AUX(N-4,I)+1.333333*H*(AUX(N+6,I)+AUX(N+6,I)-AUX(N+5,I)+
   1AUX(N+4,I)+AUX(N+4,I))
    Y(I)=DELT-.9256198*AUX(16,I)
207 AUX(16,I)=DELT
    CALL FCT(X,Y,DERY)
    DO 208 I=1,NDIM
   0DELT=.125*(9.*AUX(N-1,I)-AUX(N-3,I)+3.*H*(DERY(I)+AUX(N+6,I)+
   1AUX(N+6,I)-AUX(N+5,I)))
    AUX(16,I)=AUX(16,I)-DELT
208 Y(I)=DELT+.07438017*AUX(16,I)
    DELT=0.
    DO 209 I=1,NDIM
209 DELT=DELT+AUX(15,I)*ABS(AUX(16,I))
    IF(DELT-PRMT(4))210,222,222
210 CALL FCT(X,Y,DERY)
    CALL OUTP(X,Y,DERY,IHLF,NDIM,PRMT)
    IF(PRMT(5))212,211,212
211 IF(IHLF-11)213,212,212
212 RETURN
213 IF(H*(X-PRMT(2)))214,212,212
214 IF(ABS(X-PRMT(2))-.1*ABS(H))212,215,215
215 IF(DELT-.02*PRMT(4))216,216,201
216 IF(IHLF)201,201,217
217 IF(N-7)201,218,218
218 IF(ISTEP-4)201,219,219
219 IMOD=ISTEP/2
    IF(ISTEP-IMOD-IMOD)201,220,201
220 H=H+H
    IHLF=IHLF-1
    ISTEP=0
    DO 221 I=1,NDIM
    AUX(N-1,I)=AUX(N-2,I)
    AUX(N-2,I)=AUX(N-4,I)
    AUX(N-3,I)=AUX(N-6,I)
```

```
      AUX(N+6,I)=AUX(N+5,I)
      AUX(N+5,I)=AUX(N+3,I)
      AUX(N+4,I)=AUX(N+1,I)
      DELT=AUX(N+6,I)+AUX(N+5,I)
      DELT=DELT+DELT+DELT
 2210AUX(16,I)=8.962963*(Y(I)-AUX(N-3,I))-3.361111*H*(DERY(I)+DELT
    1+AUX(N+4,I))
      GOTO 201
  222 IHLF=IHLF+1
      IF(IHLF-10)223,223,210
  223 H=.5*H
      ISTEP=0
      DO 224 I=1,NDIM
     0Y(I)=.00390625*(80.*AUX(N-1,I)+135.*AUX(N-2,I)+40.*AUX(N-3,I)+
     1AUX(N-4,I))-.1171875*(AUX(N+6,I)-6.*AUX(N+5,I)-AUX(N+4,I))*H
     0AUX(N-4,I)=.00390625*(12.*AUX(N-1,I)+135.*AUX(N-2,I)+
     1108.*AUX(N-3,I)+AUX(N-4,I))-.0234375*(AUX(N+6,I)+18.*AUX(N+5,I)-
     29.*AUX(N+4,I))*H
      AUX(N-3,I)=AUX(N-2,I)
  224 AUX(N+4,I)=AUX(N+5,I)
      X=X-H
      DELT=X-(H+H)
      CALL FCT(DELT,Y,DERY)
      DO 225 I=1,NDIM
      AUX(N-2,I)=Y(I)
      AUX(N+5,I)=DERY(I)
  225 Y(I)=AUX(N-4,I)
      DELT=DELT-(H+H)
      CALL FCT(DELT,Y,DERY)
      DO 226 I=1,NDIM
      DELT=AUX(N+5,I)+AUX(N+4,I)
      DELT=DELT+DELT+DELT
     0AUX(16,I)=8.962963*(AUX(N-1,I)-Y(I))-3.361111*H*(AUX(N+6,I)+DELT
     1+DERY(I))
  226 AUX(N+3,I)=DERY(I)
      GOTO 206
      END


C THE FOLLOWING IS THE SUBROUTINE WHICH DEFINES THE EQUATIONS TO BE
C INTEGRATED AND THEIR ASSOCIATED VARIABLES.
      SUBROUTINE FCT(X,Y,DERY)
      REAL M,N,K1,K2,I,L,J
      DIMENSION Y(4),DERY(4)
      IF(X)20,10,20
   10 READ,U,T,P,Q,N,M
      PRINT5,N,M,U,T,P,Q
    5 FORMAT('1',5X,'N =',F10.5,2X,'M =',F10.5,2X,'U =',F10.5,2X,'T =',
     1F10.5,2X,'P =',F10.5,2X,'Q =',F10.5)
      PRINT7
    7 FORMAT('0',5X,'X',11X,'VEL',9X,'TEM',9X,' P1 ',8X,' P2 ',8X,
```

```
      1' Q1 ',8X,' Q2 ',8X,' T1 ',8X,' T2 ')
       L=1.
       PR1=30.E+25
       QR1=10.E+25
       W=(M*L)/(T*(U**2))
       PR2=(P*PR1)/(N*M*(U**2))
       QR2=(Q*QR1)/(M*N*(U**3))
       B=SQRT(.5*(M+1.))
       A=M+1.
       H=PR1/((U**2)*PR2)
       I=QR1/((U**2)*PR2)
       J=QR1/PR1
       Z=QR2/PR1
       ZZ=QR2/PR2
       E=B/N
       ART=((1.-U)/U)**2
       ART1=(2.*M*B)/(A**2)
       A1=B*(M*N+1.)/(A*N)
       A2=ART1*(N+1.)/N
       B1=2.*B*(N*L*((M*U)**2)-W)/(W*N *L*(A**2))
       B2=B1*ART
       C1=B2/(A2-2.*A1)
       C2=((1.-T)/T)    -C1
       C3=(B*(M*C1+ART/L))/(A1*N*(A**2))
       C4=(ART1*C2)/(N*A2)
       C5=1.+C3+C4
    20 EX1=-A1*X
       EX2=-A2*X
       C=(SQRT(ART))*EXP(EX1)
       D=U*C
       F=C1*EXP(2.*EX1)+C2*EXP(EX2)
       Y3=-C3*EXP(2.*EX1)-C4*EXP(EX2)+C5
       Y4=T*(F+Y3)
       G=Y4-T*Y3
       DERY(1)=-.775*Y(1)+( .45*B/(N*(A**2)))          *((1.-4.444*A)*Y(1)
      1+H*Y(2)+.667*PR1*(C**2))
       DERY(2)=(-.775*(SQRT(M))*Y(2)/N)+.45*B*((M/A)**2)*((1.-4.444*A/M)*
      1Y(2)+(Y(1)/H)+.667*PR2*(D**2))
       DERY(3)=-.508*Y(3)+(2.*E/(A**3))    * (((N*M*Y(4))/Q)-(.968-1.968
      1*A+1.5*(A**2))*Y(3)+1.936*I*C*Y(2)+2.*J*C*(.968-1.742*A+.5*(A**
      22))  *Y(1)+QR1*C*(.968*(C**2)+1.613*L*M*F+.833*L*(A**2)*Y3   ))
       DERY(4)=(-.508/N)*(SQRT(M))*Y(4)+2.*B*((M/A)**3)*(((Q*Y(3))/(M*N))
      1-(.968-1.968*(A/M)+1.5*((A/M)**2))*Y(4)-1.936*Z*(U**2)*D*Y(1)
      2-2.*ZZ*D*(.968-1.742*(A/M)+.5*((A/M)**2))*Y(2)-QR2*D*(.968*
      3(D**2)+1.613*(W/M)*(-G)+.833*W*((A/M)**2)*Y4   ))
       RETURN
```

```
C THE FOLLOWING ARE THE SUBROUTINES WHICH CONTROL THE OUTPUT OF THE
C PROGRAM.

C THIS IS VERSION I OF THE SUBROUTINE OUTP.
      SUBROUTINE OUTP(X,Y,DERY,IHLF,NDIM,PRMT)
      REAL M,N
      DIMENSION Y(4),DERY(4),PRMT(5),SA(9)
      IF(X)31,41,31
   31 SA(2)=X
      GO TO 131
   41 READ,U,T,N,M,PR
      JIP=1
      JAY=1
      MAY=1
      LAY=1
      NAY=1
      KAY=1
      IAY=1
      L=2.
      PR1=30.
      QR1=10.
      W=(M*L)/(T*(U**2))
      A=M+1.
      B=SQRT(.5*(M+1.))
      ART=((1.-U)/U)**2
      ART1=(2.*M*B)/(A**2)
      A1=B*(M*N+1.)/(A*N)
      A2=ART1*(N+1.)/N
      B1=2.*B*(N*L*((M*U)**2)-W)/(W*N *L*(A**2))
      B2=B1*ART
      C1=B2/(A2-2.*A1)
      C2=((1.-T)/T)   -C1
  131 EX1=-A1*X
      EX2=-A2*X
      C=(SQRT(ART))*EXP(EX1)
      VEL=-C
      F=C1*EXP(2.*EX1)+C2*EXP(EX2)
      TEM=-F
      IF(X)211,20,211
   20 SA(9)=X
      EVEL=VEL/2.71828
      ETEM=TEM/2.71828
      EP1=Y(1)/2.71828
      EP2=Y(2)/2.71828
      EQ1=Y(3)/2.71828
      EQ2=Y(4)/2.71828
C. THE FOLLOWING SERIES OF IF-STATEMENTS DETERMINES WHETHER OR NOT
C A QUANTITY HAS REACHED 1/E OF ITS INITIAL VALUE.
  211 IF(JAY)21,29,21
   21 IF(EVEL-VEL)22,23,23
```

```
 22 SA(9)=X
    GO TO 29
 23 XVEL=(SA(9)+X)/2.
    PRINT600,XVEL
600 FORMAT('  HOORAY!!   Z11(VEL) =',F12.6)
    JAY=0
 29 IF(LAY)50,55,50
 50 IF(EP1-Y(1))53,54,54
 53 SA(9)=X
    GO TO 55
 54 XP1=(SA(9)+X)/2.
    PRINT602,XP1
602 FORMAT('  HOORAY!!   Z11(P1) =',F12.6)
    LAY=0
 55 IF(NAY)56,60,56
 56 IF(EP2-Y(2))58,59,59
 58 SA(9)=X
    GO TO 60
 59 XP2=(SA(9)+X)/2.
    PRINT603,XP2
603 FORMAT('  HOORAY!!   Z11(P2) =',F12.6)
    NAY=0
 60 IF(KAY)61,65,61
 61 IF(EQ1-Y(3))63,64,64
 63 SA(9)=X
    GO TO 65
 64 XQ1=(SA(9)+X)/2.
    PRINT604,XQ1
604 FORMAT('  HOORAY!!   Z11(Q1) =',F12.6)
    KAY=0
 65 IF(IAY)66,72,66
 66 IF(EQ2-Y(4))69,70,70
 69 SA(9)=X
    GO TO 72
 70 XQ2=(SA(9)+X)/2.
    PRINT605,XQ2
605 FORMAT('  HOORAY!!   Z11(Q2) =',F12.6)
    IAY=0
 72 IF(JAY)71,74,71
 74 IF(LAY)71,75,71
 75 IF(NAY)71,76,71
 76 IF(KAY)71,77,71
 77 IF(IAY)71,78,71
578 X=X+.01
    EX1=-A1*X
    EX2=-A2*X
    F=C1*EXP(2.*EX1)+C2*EXP(EX2)
    TEM=-F
 78 IF(ETEM-TEM)27,28,28
 27 SA(9)=X
    GO TO 578
```

```
 28 XTEM=(SA(9)+X)/2.
    PRINT601,XTEM
601 FORMAT('  HOORAY!!   Z11(TEM) =',F12.6)
    PRMT(5)=1.
C THE FOLLOWING CALCULATES THE RATIOS OF THE RESPECTIVE
C Z11'S TO Z11 FOR THE TEMPERATURE DIFFERENCE.
    RXVE=XVEL/XTEM
    RXP1=XP1/XTEM
    RXP2=XP2/XTEM
    RXQ1=XQ1/XTEM
    RXQ2=XQ2/XTEM
    PRINT998
998 FORMAT(' THE RATIOS OF THE RESPECTIVE Z11S TO Z11(TEM) ARE')
    PRINT999,RXVE
999 FORMAT(' RZ11(VEL) =',F12.6)
    PRINT991,RXP1
991 FORMAT(' RZ11(P1) =',F12.6)
    PRINT992,RXP2
992 FORMAT(' RZ11(P2) =',F12.6)
    PRINT993,RXQ1
993 FORMAT(' RZ11(Q1) =',F12.6)
    PRINT994,RXQ2
994 FORMAT(' RZ11(Q2) =',F12.6)
    GO TO 371
 71 IF(X)67,151,67
 67 XD=SA(2)-SA(1)
    IF(XD-PR)371,151,151
151 SA(1)=X
    DM=(M+1)/2.
    XN=X/N
C THE FOLLOWING DETERMINES THE VARIOUS COLLISION FREQUENCIES.
    Z12=(SQRT(DM))*XN
    Z21=(SQRT(DM))*X
    Z22=(SQRT(M))*XN
    PRINT5,IHLF,PRMT(3)
  5 FORMAT(' ',' IHLF = ',I3,' INCREMENT =',F12.6)
C HERE THE DEPENDENT AND INDEPENDENT VARIALBLES AND THE COLLISION
C FREQUENCIES ARE PRINTED IN THEIR DESIRED FORM.
    PRINT6,X,VEL,TEM,Y(1),Y(2),Y(3),Y(4),Z12,Z21,Z22
  6 FORMAT(10F12.6)
132 IF(X)133,271,133
133 SA(1)=SA(2)
271 SA(9)=X
171 GO TO(134,234,371),JIP
134 IF(X-9.999)371,33,33
 33 PRMT(3)=.01
    PRMT(4)=.0001
    PR=4.999
    JIP=2
    GO TO 371
```

```
234 IF(X-95.00)371,534,534
534 PRMT(3)=.1
    PRMT(4)=.0001
    PR=49.99
    JIP=3
    GO TO 371
371 CONTINUE
    RETURN
    END

C THIS IS VERSION II OF THE SUBROUTINE OUTP.
    SUBROUTINE OUTP(X,Y,DERY,IHLF,NDIM,PRMT)
    REAL M,N
    DIMENSION Y(4),DERY(4),PRMT(5),SA(9)
    IF(X)31,41,31
 31 SA(2)=X
    XD=SA(2)-SA(1)
    IF(XD-PR)71,51,51
 41 READ,U,T,N,M,PR
    L=1.
    W=(M*L)/(T*(U**2))
    A=M+1.
    B=SQRT(.5*(M+1.))
    ART=((1.-U)/U)**2
    ART1=(2.*M*B)/(A**2)
    A1=B*(M*N+1.)/(A*N)
    A2=ART1*(N+1.)/N
    B1=2.*B*(N*L*((M*U)**2)-W)/(W*N *L*(A**2))
    B2=B1*ART
    C1=B2/(A2-2.*A1)
    C2=((1.-T)/T)   -C1
    C3=(B*(M*C1+ART/L))/(A1*N*(A**2))
    C4=(ART1*C2)/(N*A2)
    C5=1.+C3+C4
 51 SA(1)=X
    EX1=-A1*X
    EX2=-A2*X
    C=(SQRT(ART))*EXP(EX1)
    VEL= C
    F=C1*EXP(2.*EX1)+C2*EXP(EX2)
    TEM=-F
    Y3=-C3*EXP(2.*EX1)-C4*EXP(EX2)+C5
    Y4=T*(F+Y3)
    Y1=Y(1)*1.E-25
    Y2=Y(2)*1.E-25
    Y33=Y(3)*1.E-25
    Y44=Y(4)*1.E-25
    PRINT5,IHLF,PRMT(3)
```

```
      5 FORMAT(' ',' IHLF = ',I3,' INCREMENT = ',F12.6)
C HERE THE DEPENDENT AND INDEPENDENT VARIABLES ARE PRINTED IN
C THEIR DESIRED FORM.
        PRINT6,X,VEL,TEM,Y1,Y2,Y33,Y44,Y3,Y4
      6 FORMAT(10F12.6)
        IF(X)67,71,67
     67 SA(1)=SA(2)
     71 CONTINUE
        RETURN
        END
```