VERTICAL DISTRIBUTION
OF VIBRATIONAL ENERGY
OF MOLECULAR NITROGEN IN A STABLE
AURORAL RED ARC AND ITS EFFECT
ON IONOSPHERIC ELECTRON DENSITIES

GEORGE P. NEWTON

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by

George P. Newton

Washington, D.C.
1972
This dissertation was approved by 

as director and by 

and

as readers.
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ABSTRACT

Previous solutions of the problem of the distribution of vibrationally excited molecular nitrogen in the thermosphere have either assumed a Boltzmann distribution and considered diffusion as one of the loss processes or solved for the energy level populations and neglected diffusion. This work combines both of the previous approaches by solving the time dependent continuity equations, including the diffusion process, for the first six energy levels of molecular nitrogen for conditions in the thermosphere corresponding to a stable auroral red arc. The primary source of molecular nitrogen excitation was subexcitation, inelastic, collisions between thermal electrons and molecular nitrogen. The reaction rates for this process were calculated from published cross section calculations. The loss processes for vibrational energy were electron and atomic oxygen quenching and vibrational energy exchange. The coupled sets of non-linear, partial differential equations were solved numerically by employing finite difference equations. The results show that molecular nitrogen in excited vibrationally to the degree that the rate constant for the rate limiting ionospheric loss process $O^+ + N_2 \rightarrow NO^+ + N$ is increased by as much as a factor of eight at $F_2$ region altitudes. It was found that deviations from a Boltzmann distribution caused the reaction rate constant to be as much as 1.7 times the reaction rate constant calculated for the energetically equivalent Boltzmann distributed densities.
The time constant for loss of ionospheric electrons was calculated using the enhanced reaction rates. It was found that, for altitudes where the normal loss time constant is less than one day, the loss time constant was decreased in the arc by factors of 1.6 to 5 depending on altitude. It is concluded that the observed decrease of electron density in the $F_2$ region in stable auroral red arcs can be explained by enhanced reaction rates for ion-atom interchange between $O^+$ and $N_2$ caused by vibrational excitation of molecular nitrogen through electronic collisions.
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CHAPTER I. INTRODUCTION

1.1 Description of Stable Auroral Red Arcs

Stable Auroral Red Arcs (SAR-Arcs) are photometrically observed enhancements of air-glow at 6300 Å and 6364 Å wavelengths occurring during geomagnetically active times. They were first observed by Barbier (1) in 1957. The emissions are from the forbidden red lines of atomic oxygen OI (^1D→^3P). Peak intensities of emissions are located at altitudes near 400 km. and vary from a few hundred rayleighs to tens of kilorayleighs. The arcs generally occur near midlatitudes and are distinct in location from usual auroral phenomena. They extend over spatial dimensions of approximately 1000 km. horizontally in a meridional direction and globally in a longitudinal direction. The arcs are magnetically controlled as evidenced by their alignment in geomagnetic, rather than geographic latitude, and by their simultaneous occurrence at magnetically conjugate points. Once the SAR-arc is formed it generally persists for ten hours or longer. The frequency of observation appears to follow the solar cycle. Reviews of the general properties of SAR-arcs and citations to the literature are contained in Reference (2) and more recently Reference (3).

1.2 Cause of SAR-Arcs

The absence of the atomic oxygen green line OI (^1S→^1D) in the air glow enhancements during SAR-arcs, implies that a low energy source must exist for the excitation of the OI(^1D) state. Several mechanisms have been proposed for selectively exciting ^1D level and their implications studied (see (3) for summary).

\[^1\text{a rayleigh is } 10^6 \text{ photons cm}^{-2} \text{ sec}^{-1}\]
but one proposal has recently gained prominence. In this proposal (4) energy originating in the solar wind is transferred through the ring current in the magnetosphere to the ambient plasma, from which it is conducted down magnetic field lines into the ionosphere where it heats ambient electrons. These heated electrons collisionally excite the atomic oxygen $^1D$ level, but lack sufficient energy to excite the $^1S$ level. This proposal was utilized together with in-situ measurements of electron temperatures and densities by Roble et al. (5), (6) who found it to be consistent with all observations. Other proposals have been excluded by in-situ measurements (see (3) for discussion of the proposals and (7), (8) for observations).

1.3 Ionospheric Behavior in a SAR-ARC

From ground based (see (3) for review) and more importantly from satellite obtained data (9), (6), (7), (8), the following behavior of the ionosphere in the vicinity of SAR-arc has been determined.

At the satellites where the electron temperatures, and in some instances the ion temperatures, were measured a general enhancement of the charged particle temperatures was observed on the geomagnetic field lines intersecting the SAR-arcs. The electron densities at these satellite attitudes (usually greater than 1000 km.) showed for different SAR-arc occurrences both increases, decreases and no change in the electron densities, apparently depending on the altitude of measurement. However, corresponding topside sounder data always showed electron density depressions in the lower $F_2$ regions (near 300–800 km altitude) in the corresponding region of enhanced electron temperature. The electron density scale heights often are less in the red arc region, reflecting changes in the ion composition (7), (6). The more complex electron density behavior at the
higher altitudes (1000 km and greater) may in part be explained by a combination of the ion composition changes and the increased plasma temperature. A typical observation of the electron density and temperature in the vicinity of a SAR-arc is shown in Figure 1-1.

1.4 Objective of this work

One of the primary loss processes for ionization in the $F_2$ region, where atomic oxygen ions are the dominate ion species, is

$$\text{O}^+ + \text{N}_2 \overset{k}{\longrightarrow} \text{NO}^+ + \text{N}$$  \hspace{1cm} (1-1)

followed by

$$\text{NO}^+ + \text{e} \overset{a}{\rightarrow} \text{N} + \text{O}$$  \hspace{1cm} (1-2)

where $k$ and $a$ are the ion-atom interchange and dissociative recombination reaction rates, respectively. Typically $a$ is about four orders of magnitude greater than $k$, (11), so that the rate determining process for ionization loss is reaction (1-1). However, $k$ in reaction (1-1) is known to be a strong function of the vibrational temperature of molecular nitrogen (12), (13). This is why knowledge of the energy distribution of the excited levels plays a crucial role in the understanding of the electron loss rates in the SAR-arc. Thus, as suggested earlier, (12), the loss of ionospheric ionization may be considerably enhanced by the presence of vibrationally excited nitrogen. The source of the vibrationally excited nitrogen molecules is sub-excitation,\(^2\) inelastic, collisions between the

\(^2\)Subexcitation means that the final state of the $\text{N}_2$ is neither electronically excited nor ionized.
Figure 1-1. Observed ionospheric electron densities and observed and calculated electron temperatures for a 500 R SAR-arc.
Figure 1-2. Model neutral atmosphere and ionospheric electron densities
Figure 1-3. Neutral atmosphere kinetic and electron temperature models
ambient molecular nitrogen and the thermal ionospheric electrons, the same mechanism that excites the OI(1D). The cross section for this type of process is important to this study (Appendix I).

The objective of this work is to investigate the distribution of vibrationally excited molecular nitrogen under conditions corresponding to a SAR-ARC to determine if the presence of vibrationally excited nitrogen can account for the observed decrease in the electron density in the $F_2$ region. For this study we used the same electron density profiles that Roble (10) used to calculate the temperature profiles for SAR-arcs, and we used his calculated electron temperatures. The electron density profile and model atmosphere used for this work are shown in Figure 1-2. The neutral atmospheric model used for this work is the 1965 Jacchia model (14) with an exospheric temperature of 1500°K. We did not include minor constituents. The neutral atmosphere temperature profile is shown in Figure 1-3, together with several of Robel's, (10), electron temperature profiles corresponding to different SAR-ARC intensities.
2.1 Previous Calculations of the Distribution of Vibrationally Excited Nitrogen

Several authors have suggested that vibrationally excited nitrogen may influence the excitation of atmospheric radiations, chemical reactions, and the ionospheric temperature (15), (16), (17), (18), (12), (19). Walker et. al. (20) were the first to calculate the altitudinal distribution and diurnal variation of the vibrating molecules assuming a Boltzmann distribution. The diurnal calculations assumed an unperturbed atmosphere and ionosphere. They considered diffusion of the vibrationally excited nitrogen vertically and limited their calculation to altitudes between 100 km and 300 km altitude. They found that vibrational energy exchange with CO$_2$ was the dominant loss process for vibrational quanta below 125 km altitude. The principal sources of vibrational quanta in the lower thermosphere (100 km and 600 km) were found to be: (1) the reaction between atomic nitrogen and nitric oxide; (2) the collisions of photoelectrons and nitrogen molecules; and (3) possibly the quenching of metastable oxygen atoms, O$_1$($^1$D), by nitrogen, although the vibrational yield of the last process is unknown.

Recently, McNeal, et. al. (21) measured the reaction rate for vibrational-translation energy exchange between atomic oxygen and vibrationally excited molecular nitrogen at 300°K and found the rate to be considerably larger than extrapolated values (which were used by Walker et. al. (20).) obtained from experiments at higher temperatures. The quenching of vibrationally excited molecular nitrogen by atomic oxygen, which was ignored in the calculations of Walker et. al. (20), has been included in the calculations of Breig, et. al (22) who used the recently determined reaction rate. They essentially repeated the calculations
of Walker, et al. (19) and found that inclusion of the loss of vibrational excitation by nitrogen molecules to atomic oxygen significantly decreased (by factors of 2 to 4) the vibrational temperatures in the lower thermosphere.

Schunk and Hays (23) solved the continuity equations for the first eleven energy levels of molecular nitrogen for altitudes above 150 km. under conditions corresponding to an aurora. Diffusion processes were not included in their calculations. The source of vibrational excitation was non-thermal electrons and the only loss process included for each level was vibrational energy exchange between nitrogen molecules. They found that when the non-thermal electron source was acting, the \( \text{N}_2 \) vibrational distribution was non-Boltzmann and that the deviation from the Boltzmann distribution increased with increasing altitude. They found that the loss rate for \( \text{O}^+ \) due to reaction (1-1) was increased by a factor of 1.5 when allowance was made for the non-Boltzmann distribution. The non-thermal electron source was allowed to operate for 15 min. and they found that the enhanced loss rate persisted for 1000-2000 sec. after the auroral bombardment commenced.

Walker (24) discussed the result of Schunk and Hays (23) and included in his discussion the effects of diffusion. He starts with the steady state continuity equation for each level and ignores quenching processes for the vibrationally excited nitrogen molecules. Under these conditions, the source of vibrational excitation and diffusion are the only terms which can cause departures from a Boltzmann distribution. By comparing the production term for a given vibrational level with the production at that level due to vibrational exchange, he concluded that departures for vibrational levels containing a significant fraction of the nitrogen molecules will not exist at altitudes below 300 km. By comparing the diffusive
flux term with the loss due to vibrational energy exchange he concludes that diffusion is less important than vibrational energy exchange at altitudes below 370 km. These conclusions were based on conditions of an undisturbed atmosphere and source terms similar to those used by Walker, et al. (20).

2.2 Differences between this and previous works.

The source of vibrational excitation for this work is the thermal electrons in SAR-arcs. This source extends to higher altitudes than the sources used by Walker, et. al (20), Breig et. al., (22) and Schunk and Hays (23). As a result, the molecular excitation occurs in a region of the thermosphere where vibrational energy exchange is slow in comparison with the diffusion process. Thus, because the source is non-Boltzmann in its energy distribution and because the excited molecules diffuse to lower altitudes where vibrational energy exchange is the dominant process, the assumptions of a Boltzmann distribution and negligible diffusion loss are no longer tenable. This work differs from that of Walker, et. al., (20) and Breig, et. al. (22), by not assuming a Boltzmann distribution, and from that of Schunk and Hays (23) by including diffusion of the excited molecules.

2.3 The equations of continuity.

The continuity equation for each energy level of vibrationally excited molecular nitrogen, $N_2^*$, governs the level population and its altitudinal distribution. For the $i$th level the equation is

$$\frac{\partial}{\partial t} n_i + \nabla \cdot (n_i \bar{v}_i) = Q_i - L_i \quad (2-1)$$
where \( n_i \) is the number density of molecular nitrogen in energy level \( i \)

\[ \vec{v}_i \] is the vector velocity of transport of \( n_i \)

\( Q_i \) is the production rate of \( n_i \)

\( L_i \) is the loss rate of \( n_i \).

In principal the production and loss rate terms contain all sources and sinks for the \( i \)th level. However, we are interested in solutions of (2-1) corresponding to SAR-arc conditions where the electron temperature is unusually large. In addition we are interested in a process which, to first order, can be considered as an additional source to those ordinarily present in the thermosphere.

Figure 2-1 shows the rates of the dominant processes for equation (2-1). Also included in Figure 2-1, for comparison purposes, are the total vibrational quanta production rates between 120 and 300 km, calculated from the work of Walker et al. (20) and Kummuler and Bortner (25) and shown as squares and circles, respectively. Shown as triangles in Figure 2-1 are the CO\(_2\) quenching rates for vibrationally excited nitrogen at 120 km, taken from references (20), (22) and (25).

The atomic oxygen quenching curve shown in Figure 2-1 was calculated using the reaction rate of \( 3.5 \times 10^{-15} \text{ cm}^3\text{sec}^{-1} \), (21), and the atomic oxygen number density shown in Figure 1-2. The curve of atomic oxygen production of \( N_2^* \) (translational-vibrational energy exchange process) was calculated from the quenching curve using detailed balance considerations. These curves correspond to \( 1 \rightarrow 0 \) and \( 0 \rightarrow 1 \) transitions of \( N_2 \) respectively.

The vibrational energy exchange curve was calculated for the \( 0 \rightarrow 1, 1 \rightarrow 0 \) transitions using the exact resonance case of the Schwartz-Slawsky-Herzfeld,
(SSH), theory, (27) page 330, and the molecular nitrogen number density profile of Figure 1-2.

The rate for diffusion was calculated from the diffusion coefficient, $D$, and the density scale height, $H$, for molecular nitrogen by

$$\text{rate} = \frac{D}{H^2}$$

This rate may be regarded as the inverse of the time for a nitrogen molecule to diffuse to an altitude where there is an appreciably greater density (by a factor of $e$) of molecular nitrogen.

The electronic production curve was calculated using the reaction rates for inelastic collisions between thermal electrons and molecular nitrogen discussed in Appendix I and the electron and molecular nitrogen densities and electron temperatures in Figures 1-2 and 1-3, respectively. The electron temperature used is that for a 17.7 KR SAR-arc. For the calculation it was assumed that the vibrational temperature was zero.

From Figure 2-1 it is seen that the source of vibrational energy from thermal electrons, under the SAR-ARC condition, is larger over most of the altitude range of interest than the source of vibrational energy from ordinary ionospheric processes (20), (25). Because of the uncertainty in the yield of vibrational energy from $0 \left(^1D\right)$ quenching by molecular nitrogen (20), (25), and because the $O \left(^1D\right)$ density during SAR-arcs is enhanced and its spatial distribution is complex, we have ignored this potential source term. Thus, the source term, $Q_i$, in equation (2-1) will only include production of vibrationally excited nitrogen by collisions between nitrogen molecules and thermal electrons (and only
coincidently by atomic oxygen) and vibrational energy exchange between nitrogen molecules. These approximations should underestimate the source terms and hence the calculated temperatures would tend to be a lower bound for this reason.

The dominant loss processes for vibrationally excited molecular nitrogen at higher altitudes is electron quenching at altitudes above 400 km. (20, 25), and diffusion above 320 km. (see Figure 2-1). At low altitudes the dominant loss processes are quenching by atomic oxygen for altitudes between 120 and 300 km (Walker et al., (20), found that quenching by other minor constituents in the lower thermosphere through translational-vibration energy exchange was negligible) and vibrational energy exchange with $CO_2$ (20), (22), at 120 km. Thus, the loss term, $L_i$, in equation (2-1) will include loss by electron and atomic oxygen quenching and vibrational energy exchange with molecular nitrogen. The vibrational energy loss by molecular nitrogen to carbon dioxide will be included through a lower boundary condition on the vibrational temperature for the following reasons. The abundance of carbon dioxide at 120 km is somewhat uncertain and depends on the altitude of the turbopause. The turbopause of the atmosphere is below 120 km altitude. Thus, in the altitude region of interest, carbon dioxide could be expected to approach diffusive equilibrium. Because of its relatively large mass, the density of carbon dioxide should decrease rapidly above 120 km. and increase rapidly below 120 km. altitude, thus creating a loss process significant only at the lower boundary.
The source and loss terms for equation (2-1) are therefore given by

\[ Q_i = \sum_{j=0}^{i-1} A_{i,j} n_j + \sum_{j=0}^{i-1} P_{i,j;i-1,j+1} n_{j+1} \]

\[ + \sum_{j=1}^{i} P_{i,j+1;i-1,j} n_{j+1} n_{j-1} + C_{i,i-1} \nu_{i-1,[0]} n_{i-1} \]

\[ + C_{i,i+1} \nu_{i+1,[0]} n_{i+1} \quad (2-3) \]

\[ L_i = \sum_{j=0}^{i-1} A_{j,i} n_i + \sum_{j=0}^{i-1} P_{i-1,j+1;i,i} n_j \]

\[ + \sum_{j=1}^{i} P_{i+1,j-1;i,j} n_{i-1} \]

\[ + C_{i-1,i} \nu_{i,[0]} + C_{i+1,i} \nu_{i,[0]} n_i \quad (2-4) \]

where a prime on the summation excludes \( j = i \), and

\( P_{i,j;i-1,j+1} \) is the exchange transition probability for a nitrogen molecule in level \( i - 1 \) going to level \( i \) while the collisional partner molecule goes from level \( j + 1 \) to level \( j \).

\( \nu_{i,j} \) is the collision frequency of a nitrogen molecule in level \( j \) with a molecule in level \( i \).

\( C_{i,j} \) is the probability for collisional transitions from level \( j \) to level \( i \) where the collision is with atomic oxygen atoms.

\( A_{i,j} \) is the reaction rate, from Appendix I, for the transition from level \( j \) to level \( i \) due to collisions between thermal electrons and molecular nitrogen molecules in level \( j \).
\( \nu_{i,0} \) is the collision frequency of a molecule in level \( i \) with an atomic oxygen atom.

2.4 The coefficients in the equations of continuity.

The cross sections for the subexcitation, inelastic, scattering of electrons by molecular nitrogen (28), (29), (30) are only available for the first five energy levels. These cross-section calculations and the calculation of reaction rates from the cross-sections are discussed in Appendix 1.

We will assume that molecular nitrogen can be represented by a harmonic oscillator. Thus, only transitions between adjacent levels will be considered. This assumption is appropriate for the moderate vibrational temperatures of this problem where only the lower lying energy levels are important and where anharmonic effects are small (31), (32), (33). It is also implicit to this calculation that the first five excited levels of molecular nitrogen will be considered as the totality of excited levels.

The above assumption and the theory for exact resonance vibrational-vibrational energy exchange of SSH, (27), allow us to write the vibrational-vibrational energy exchange probability in terms of the \( 0 \rightarrow 1, 1 \rightarrow 0 \) transitions of molecular nitrogen as

\[
P_{i,j:i-1,j+1} = i(j+1)P_{1,0:0,1}
\] (2-5)

From detailed balance considerations

\[
P_{i-1,j+1:i,j} = P_{i,j:i-1,j+1}
\] (2-6)
Setting the steric factor in the SSH theory to three, and using the Lennard-Jones potential parameters for \( N_2 \) from table 66-1 of (27), and table 66-5 of (27) for the characteristic \( \ell \) of the theory, we have

\[
P_{i, j: i-1, j+1} = 2.600322 \times 10^{-6} \, i (j + 1) \, T \, e^{91.5/T} \tag{2-7}
\]

where \( T \) is the kinetic gas temperature.

It is assumed that

\[
C_{i+1, i} = (i + 1) \, C_{1, 0} \tag{2-8}
\]

for the translational-vibrational energy exchange probability, the reason will become apparent later. Thus, (2-8) is consistent with SSH theory, but \( C_{1, 0} \) will not be determined from this theory (see reference (21)). Detailed balance gives

\[
C_{i, i-1} = C_{i-1, i} \, e^{-\theta/T} \tag{2-9}
\]

where \( \theta \) is the characteristic temperature of \( N_2 \) (\( \theta = 3380^\circ K \)).

We assume that the vibrational level in which the nitrogen molecule resides does not effect its collision cross section for both molecules and atoms. Thus we write

\[
\nu_{ji} = \nu n_i \tag{2-10}
\]

\[
\nu_{i, [0]} = \nu' n [0], \tag{2-11}
\]

Equations (2-3) and (2-4) become respectively

\[
Q_i = \sum_{j=0} A_{ij} \, n_j + P_{1, 0: 0, 1} \, \nu \sum_{j=0} i (j + 1) \, n_{i-1} \, n_{j+1} + P_{1, 0: 0, 1} \, \nu \sum_{j=1} j (i + 1) \, n_{i+1} \, n_{j-1} + C_{1, 0} \, \nu' \, n [0] \, [i n_{i-1} + (i + 1) \, e^{\theta/T} \, n_{i+1}] \tag{2-12}
\]

---

3 The measured reaction rate for \( C_{0, 1} \) is several orders of magnitude larger than would be calculated using SSH theory. The reason for the discrepancy may be that chemical interactions are responsible for the anomalous quenching, whereas SSH theory attributes the interaction as being due to short range repulsive potentials.
\[ L_i = \sum_{j=0}^{i} A_{ji} n_i + P_{1,0:0,1} \nu \sum_{j=0}^{i} i(j + 1) n_i n_j + P_{1,0:0,1} \nu \sum_{j=i}^{n} j(i + 1) n_j n_i + C_{1,0} \nu' n [0] [i e^{\theta/T} + (i + 1)] n_i \]  

(2-13)

The quantity \( \nu \) in equations (2-10), (2-12) and (2-13) is calculated from equation (36-3) of reference (27)

\[ \nu = \frac{1.271 \rho}{\eta_{N_2} n} \]  

(2-14)

where

\( \rho \) is the gas pressure

\( N_2 \) is the viscosity for molecular nitrogen

\( n \) is the total number density of molecular nitrogen

Using the ideal gas law, we have

\[ \nu = \frac{1.271 k T}{\eta_{N_2}} \]  

(2-15)

where \( k \) is Boltzmann's constant. Using (8.2-18) of reference (34), and average values of the appropriate parameters for temperatures of 355\(^\circ\)K and 1500\(^\circ\)K, we obtain for \( \nu \)

\[ \nu = 1.482094 \times 10^{-11} \sqrt{T} \]  

(2-16)

The quantity \( C_{1,0} \nu' \) occurring in equations (2-12) and (2-13) is calculated from \( C_{01} \nu' \) by equation (2-9), where \( C_{01} \nu' \) is considered to be a "lumped" constant equal to the reaction rate constant reported by McNeal, et. al., (21) and is considered constant with altitude.

It will be assumed that the neutral atmosphere is static, and uniform horizontally in all of its parameters. The transport velocity, \( \bar{v}_i \), is then the diffusion
velocity for molecular nitrogen through the atmosphere, and is given by (35), page 244,

\[ \vec{v}_i = -D \left[ \frac{1}{p_i} (\nabla p_i - \rho_i \vec{g}) + k_T \frac{1}{T} \nabla T \right] \]  \hspace{1cm} (2-17)

where

- \( D \) is the binary diffusion coefficient for molecular nitrogen, assumed to be independent of vibrational excitation.
- \( p_i \) is the pressure of the molecular nitrogen in energy level \( i \).
- \( \rho_i \) is the mass density of molecular nitrogen
- \( k_T \) is the thermal diffusion ratio
- \( \vec{g} \) is the acceleration of gravity.

Using the ideal gas law in (2-17) we have

\[ \vec{v}_i = -D \left[ \frac{1}{n_i} \nabla n_i + (k_T + 1) \frac{1}{T} \nabla T + \frac{mg \hat{k}}{kT} \right] \]  \hspace{1cm} (2-18)

where \( \hat{k} \) is a unit vector in the vertical direction

- \( m \) is the mass of molecular nitrogen.

Rewriting (2-18) we have

\[ \vec{v}_i = -D \left[ \frac{1}{n_i} \nabla n_i + \frac{1}{H} \hat{k} \right] \]  \hspace{1cm} (2-19)

where

\[ \frac{1}{H} = (k_T + 1) \frac{1}{T} \frac{\partial T}{\partial z} + \frac{mg}{kT} \]  \hspace{1cm} (2-20)

and \( z \) is the vertical coordinate, positive upward and \( H \) is the density scale height.

Thermal diffusion for molecular nitrogen is small, and therefore \( k_T \) will be set to zero. The flux term in equation (2-1) becomes

\[ \vec{F}_i = n_i \vec{v}_i = -D \left[ \nabla n_i + \frac{n_i}{H} \hat{k} \right] \]  \hspace{1cm} (2-21)
It will be assumed that the magnetic field line is vertical, so that the SAR-arc is symmetrical about the vertical. Under this assumption the horizontal flux at the arc center vanishes. If, in addition, the divergence of the horizontal flux is ignored, equation (2-1) can be reduced to one spatial dimension corresponding to conditions at the arc center.

Under the above assumptions and using (2-21), (2-12) and (2-13), equation (2-1) becomes

\[
\frac{\partial n_i}{\partial t} + \frac{\partial}{\partial z} \left( F_i \right)_z = \sum_{j=0} \left\{ A_{ij} n_j - A_{ji} n_i \right\} + P_{1,0:0,1} \nu i \sum_{j=0} (j+1) [n_{i-1} n_{j+1} - n_i n_j] - n_i n_j] + P_{1,0:0,1} \nu (i + 1) \sum_{j=1} j [n_{i+1} n_{j-1} - n_i n_j]
\]

\[
+ C_{1,0} \nu' n[0] [i n_{i-1} + (i + 1) e^{\theta/T} n_{i+1} - (i e^{\theta/T} + i + 1) n_i]
\]

(2-22)

2.5 **Boundary conditions.**

Two sets of boundary conditions will be used for equation (2-22).
For the first set we have

Initial condition: \( n_i(z, 0) = 0 \) for all \( i > 0 \)

\[ = n \text{ for } i = 0 \]

Lower boundary: \( n_i(120, t) = 0 \) for all \( i > 0 \)

\[ = n(120) \text{ for } i = 0 \]

Upper Boundary:

\[ \frac{\partial n_i}{\partial z} \bigg|_{z=\infty} = - \frac{n_i(\infty, t)}{H} \text{ for all } i. \]

The initial and lower boundary conditions correspond to all molecular nitrogen being in the ground state. This would correspond to total quenching by \( \text{CO}_2 \) at the lower boundary, and no excitation initially. The upper boundary condition insures zero flux, for all excited levels, at the top of the atmosphere.

For the second set of boundary conditions,

Initial Condition \( n_i(z, 0) = \frac{n}{1 - e^{-\theta/355}} e^{-i \theta/355} \) for all \( i \)

Lower Boundary \( n_i(120, t) = \frac{n}{1 - e^{-\theta/355}} e^{-i \theta/355} \) for all \( i \)

Upper boundary \( \frac{\partial n_i}{\partial z} \bigg|_{z=\infty} = - \frac{n_i(\infty, t)}{H} \text{ for all } i \)

The initial and lower boundary conditions in this case correspond to assuming the vibrationally excited nitrogen to be Boltzmann distributed corresponding to a vibrational temperature of 355°K, the kinetic temperature at the lower boundary.

2.6 Simplification of equations and technique of solution.

In Appendix II the set of six, coupled, non-linear, partial differential equations (2-22) are replaced by seven equations in which the essential coupling is more
readily observed. This simplification is achieved by expressing the solutions of equation (2-22) as a sum of a Boltzmann distributed part and a part representing a deviation from a Boltzmann distribution, that is

\[ n_i = n'_i + \epsilon_i \]  

(A2-1)

It is then required that the Boltzmann distributed part, \( n'_i \), possess the total vibrational energy and number density of molecular nitrogen for the problem (see equations (A2-2) and (A2-3)). The deviation part, \( \epsilon_i \), is then a measure of the departure, at each altitude, of the solution from the energetically equivalent Boltzmann solution part. The differential equation to be solved for the Boltzmann part of the solution is

\[
\frac{\partial \psi}{\partial t} - \frac{1}{n} \frac{\partial n}{\partial z} \frac{\partial \psi}{\partial z} - D \frac{\partial^2 \psi}{\partial z^2}
= \sum_{j=0}^{\infty} \sum_{i=0}^{j} \left[ \frac{1}{\psi + 1} \left( \frac{\psi}{\psi + 1} \right)^j + \frac{\epsilon_j}{n} \right] (i - j) A_{ij} \]  

(A2-30)

\[ + C_{1,0} \nu' n [0] \left[ \psi + 1 - e^{\theta/T} \psi \right] \]

where \( \psi \) is related to the partition function, \( Z_p \), for the vibrationally excited nitrogen by

\[ \psi = (Z_p - 1) \]  

(A2-27)

The differential equation for the deviation part of the solution is
\[
\frac{\partial}{\partial t} \varphi_i - D \frac{\partial^2}{\partial z^2} \varphi_i = \left[ \frac{\partial D}{\partial z} + D \left( -\frac{1}{H} + 2 \left\{ \frac{i}{\psi} - \frac{i + 1}{\psi + 1} \right\} \frac{\partial \psi}{\partial z} \right) \right] \frac{\partial \varphi_i}{\partial z} \\
+ \left\{ \left( \frac{i}{\psi} - \frac{i + 1}{\psi + 1} \right) \frac{\partial \psi}{\partial t} - \frac{\partial \psi}{\partial z} \left( \frac{i}{\psi} - \frac{i + 1}{\psi + 1} \right) \right\} \frac{\partial D}{\partial z} + D \left( -\frac{1}{H} \right) \\
+ \left\{ \left( \frac{i}{\psi} - \frac{i + 1}{\psi + 1} \right) \frac{\partial \psi}{\partial z} \right\} - D \left( \frac{i}{\psi} - \frac{i + 1}{\psi + 1} \right) \frac{\partial^2 \psi}{\partial z^2} - D \left( \frac{\partial \psi^2}{\partial z} \right) \left\{ \frac{-i}{\psi^2} \right\} \\
+ \frac{(i + 1)}{(\psi + 1)^2} \right\} + \sum_{j=0}^{n} A_{ij} (1 - \delta_{ij}) + P_{1,0:0,1} \nu n \{(2i + 1) \psi + i\} \\
+ C_{1,0} \nu' n[0] \left( i e^{\theta/T} + i + 1 \right) \varphi_i = \sum_{j=0}^{n} \left\{ A_{ij} (1 + \varphi_j) e^{-(j-1)\theta/T} \right\} (1 - \delta_{ij}) \\
- \left[ \left( \frac{i}{\psi} - \frac{i + 1}{\psi + 1} \right) \frac{\partial \psi}{\partial t} - \frac{\partial \psi}{\partial z} \left( \frac{i}{\psi} - \frac{i + 1}{\psi + 1} \right) \right\} \frac{\partial D}{\partial z} + D \left( -\frac{1}{H} \right) \\
+ \left\{ \frac{i}{\psi} - \frac{i + 1}{\psi + 1} \right\} \frac{\partial \psi}{\partial z} \right\} + \sum_{j=0}^{n} A_{ij} (1 - \delta_{ij}) - D \left( \frac{i}{\psi} - \frac{i + 1}{\psi + 1} \right) \frac{\partial^2 \psi}{\partial z^2} \\
- D \left( \frac{\partial \psi^2}{\partial z} \right) \left\{ \frac{-i}{\psi^2} + \frac{i + 1}{(\psi + 1)^2} \right\} + P_{1,0:0,1} \nu n \{(2i + 1) \psi + i\} \\
+ C_{1,0} \nu' n[0] \left( i e^{\theta/T} + i + 1 \right) + P_{1,0:0,1} \nu n \{(2i + 1) \psi + i\} \\
+ C_{1,0} \nu' n[0] \left[ i e^{\theta/T} + (i + 1) e^{\theta/T - \theta/T} \right] + \varphi_{i-1} e^{\theta/T} \left[ P_{1,0:0,1} \nu n \right] \\
+ C_{1,0} \nu' n[0] \left[ \varphi_{i+1} e^{-\theta/T} \right] + P_{1,0:0,1} \nu n (i + 1) (\psi + 1) \\
+ C_{1,0} \nu' n[0] e^{\theta/T} (i + 1) \right\} (A2-46)
where

\[ \varphi_i = \frac{\epsilon_i}{n_i} \]  \hspace{1cm} (A2-39)

The boundary conditions are

set 1:

Initial condition \( \psi(z, 0) = 0 \)

Lower boundary \( \psi(120, t) = 0 \)

Upper boundary \( \left. \frac{\partial \psi}{\partial z} \right|_{z=\infty} = 0 \) \hspace{1cm} (A2-31)

set 2:

Initial condition \( \psi(z, 0) = 7.329241 \times 10^{-5} \)

Lower boundary \( \psi(120, t) = 7.329241 \times 10^{-5} \)

Upper boundary \( \left. \frac{\partial \psi}{\partial z} \right|_{z=\infty} = 0 \) \hspace{1cm} (A2-32)

set 1 and set 2

Initial condition \( \varphi_i(z, 0) = 0 \) for all \( i \)

Lower boundary \( \varphi_i(120, t) = 0 \) for all \( i \)

Upper boundary \( \left. \frac{\partial \varphi_i}{\partial z} \right|_{z=0} = 0 \) for all \( i \) \hspace{1cm} (A2-47)

The set 1 boundary conditions on \( \psi \) correspond to a vibrational temperature initially zero, with the vibrational temperature at the lower boundary remaining zero, presumably due to quenching. The set 2 boundary conditions for \( \psi \) correspond to the initial vibrational temperature of 355°K (the kinetic temperature at the lower boundary) and the vibrational temperature at the lower boundary remaining at
$355^\circ K$. In both cases the upper boundary condition on $\psi$ corresponds to a zero flux of quanta through the top of the atmosphere.

The boundary conditions on the $\varphi_i$'s correspond to zero deviations from a Boltzmann distribution initially, with zero deviation being maintained at the lower boundary (presumably due to the rapid vibration-vibration energy exchange among $N_2$ at this altitude).

Calculation shows that the source term for vibrational quanta due to electron collisions in equation (A2–30) is only mildly non-linear (less than 30%) for the electron and vibrational temperatures of interest here. It can also be argued, that for the relatively weak source of vibrational excitation for this problem, the departures from a Boltzmann solution will be such that the term $\epsilon_j/n$ will be small relative to 1. Thus by dropping the $\epsilon_j/n$ term in (A2–30), the $\psi$ and $\varphi_i$ equations are uncoupled, and a first approximation to $\psi$ may be obtained by solving the equation

$$
\frac{\partial \psi}{\partial t} - \frac{1}{n} \frac{\partial Dn}{\partial z} \frac{\partial \psi}{\partial z} - D \frac{\partial^2 \psi}{\partial z^2} = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \left[ \frac{1}{\psi + 1} \left( \frac{\psi}{\psi + 1} \right)^j \right] (i - j) A_{ij} 
$$

$$
+ C_{1,0} \nu' n [0] [\psi + 1 - e^{\theta/T} \psi]
$$

(2-23)

When $\psi$ has been obtained, the vibrational temperature may be calculated by

$$
T_v(z, t) = \frac{\theta}{\ln \left[ \frac{\psi(z, t) + 1}{\psi(z, t)} \right]}
$$

(2-24)

and the coefficients of equations (A2–46) are known functions of altitude and time.

A first approximation to the $\varphi_i$'s can then be obtained by solving equation (A2–46).
If necessary, a second approximation to $\psi$ may be obtained from equation (A2-30) by using the first approximation of the $\varphi_i$'s to determine $\epsilon_j/n$ in the source term of equation (A2-30) and resolving equation (A2-30). A second approximation to the $\varphi_i$'s can then be obtained by using the second approximation for $\psi$ in equations (A2-46). Higher approximations may in principle be found by repeating this process.

2.7 Finite difference equations and solutions.

In Appendix III it is shown that the finite difference equations for both equations (A2-30) and (A2-46) take the general forms

\[- A_{\ell} \psi_{\ell+1}^{m+1} + B_{\ell} \psi_{\ell}^{m+1} - A_{\ell} \psi_{\ell-1}^{m+1} = D_{\ell}^m \]

(A3-7)

and

\[- C_{\ell} \psi_{\ell+1}^{m+1} + \ell_{\ell} \psi_{\ell}^{m+1} - A_{\ell} \psi_{\ell-1}^{m+1} = \ell_{\ell} \psi_{\ell}^{m+1} \]

(A3-17)

where $\ell$ refers to an altitude grid point, with $\ell = 1$ the bottom boundary and $\ell = L$ the top boundary, $m$ refers to a time grid point and $i$ refers to the energy level being solved for. The boundary conditions become for $\psi$

<table>
<thead>
<tr>
<th>set 1</th>
<th>set 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m = 1$</td>
<td>$\psi_{1}^{1} = 0$</td>
</tr>
<tr>
<td>$\ell = 1$</td>
<td>$\psi_{1}^{m} = 0$</td>
</tr>
<tr>
<td>$\ell = L$</td>
<td>$\psi_{L}^{m} - \psi_{L-1}^{m} = 0$</td>
</tr>
</tbody>
</table>
and for the \( \phi_i \)'s

\[
\begin{align*}
\ell = 1 & \quad \ell \phi_i^1 = 0 \quad \text{for all } i \\
\ell = L & \quad L \phi_i^m - L^{-1} \phi_i^m = 0 \quad \text{for all } i \quad (A3-18)
\end{align*}
\]

The two equations (A3-7) and (A3-17) are of the same form. We follow Richtmyer, (36), pages 103-104, for the solutions of (A3-7) and (A3-17). Only the solution of (A3-7) is presented here, because the extension to each of the equations in (A3-17) is clear.

It is seen that the right hand side of (A3-7) is a known quantity. Equation (A3-7) is a one parameter family, because any value of \( \psi_{2}^{m+1} \) determines a solution. Let

\[
\psi_{\ell}^{m+1} = E_\ell \psi_{\ell+1}^{m+1} + F_\ell \quad (2-25)
\]

which is also a one parameter family. We seek to find \( E_\ell \) and \( F_\ell \) such that the two families of solutions (2-25) and (A3-7) are the same. If (2-25) is to be true for any member of the family, the boundary conditions (A3-8) and (A3-9) require

\[
E_1 = 0 \quad (2-26)
\]

\[
F_1 = \begin{cases} 
0 & \text{set 1} \\
7.329241 \times 10^{-5} & \text{set 2} 
\end{cases} \quad (2-27)
\]

Substituting (2-25) into (A3-7) and placing the result in the form of (2-25) we have
Comparing equation (2-29) with (2-25) we have

\[ E_\ell = \frac{A_{\ell}}{B_{\ell} - A_{\ell} E_{\ell-1}} \quad (2-30) \]

\[ F_\ell = \frac{D_{\ell} + A_{\ell} F_{\ell-1}}{B_{\ell} - A_{\ell} E_{\ell-1}} \quad (2-31) \]

Using (2-26) and (2-27) or (2-28) we can calculate the \( E_\ell \)'s and \( F_\ell \)'s from \( 1 = 1 \) to \( 1 = L \), that is, from the lower boundary to the upper boundary, by using (2-30) and (2-31), respectively.

When \( 1 = L - 1 \), equation (2-25) gives

\[ \psi_{L-1}^{m+1} = E_{L-1} \psi_{L-1}^{m+1} + F_{L-1} \quad (2-32) \]

Using the upper boundary condition of (A3-8) or (A3-9) in (2-32) we have

\[ \psi_{L-1}^{m+1} = \frac{F_{L-1}}{1 - E_{L-1}} \quad (2-33) \]

We now repeat the process, for \( \ell = L - 2, L - 3, \ldots, 1 \), to solve for the \( \psi_{m+1}^{m+1} \)'s, that is, we solve for the \( \psi_{m+1}^{m+1} \)'s from the upper boundary to the lower boundary. This total process is repeated for each time step from \( m = 1 \) to the maximum time step of interest.

Only slight modification of this method is needed to solve for the six, coupled \( \phi_i \)'s of equation (A3-17).
The technique embodied in equations (A3-7) (A3-17) and equations (2-25) through (2-33) was programmed for the IBM 360-75 for both sets of finite difference equations (A3-7) and (A3-17). The program to solve for $\psi$ was called BOLTSOL and the program to solve for the $\phi_i$'s was called BOLTDEV. Both programs are listed in Appendix IV. Details of the numerical solutions are discussed in Chapter III.
Figure 2-1. Rates of production and loss of vibrational energy and diffusion
The finite difference equations (A3-7) and (A3-17) were solved in single precision over the altitude interval of 120 km to 920 km for conditions corresponding to those of a 17.7 KR SAR-arc, as shown in Figure 1-2 and 1-3. The upper altitude limit was lowered to 840 km, with negligible effect (less than 5° in the vibrational temperature and less than 2% in the $\phi_1$'s) on the solutions. The altitude step was taken as 40 km, and variation of the time step by a factor of 10, from 100 sec. to 10 sec. had no significant effect on the results. The solutions were generated over a time interval of 100000 seconds and approached (or reached) a steady state during that time.

Figure 3-1 shows the number of density of vibrational quanta versus altitude for a time into the solution of 95200 seconds. The number density of quanta was calculated from the solutions of equation (A3-7) corresponding to equation (2-23) (that is ignoring the $\epsilon_j/n$ term in the source term). Also shown in Figure 3-1 is the quantity $\sum_{i=0}^{\infty} i \epsilon_i$ calculated from the solutions of equations (A3-17). Theoretically equations (A2-4) and (A2-5) should be satisfied, however, because of the finite difference and other approximations, $\sum_{i=0}^{\infty} i \epsilon_i$ will not be zero. A measure of its significance is a comparison with the number of quanta calculated from the solutions of (A3-7). From Figure 3-1 it is seen that $\sum_{i=0}^{\infty} i \epsilon_i$ represents a negligible (<1%) portion of the energy in the Boltzmann solution for altitudes below 300 km. Between 300 and 600 km altitude, $\sum_{i=0}^{\infty} i \epsilon_i$ increases relative to the quantal number density, so that at altitudes of 600 km and above $\sum_{i=0}^{\infty} i \epsilon_i$ represents only about 3% of the energy of the Boltzmann solution. These conclusions are valid at all other time steps.
Figure 3-1. Comparison of $\sum_{i=0}^{\infty} \epsilon_i$ and the number density of vibrational quanta.
Figure 3-2 is a plot of $\left| \sum_{i=0}^{6} \epsilon_i / \epsilon_i \right|$ versus altitude for each of the six energy levels corresponding to a time into the solution of 94700 seconds. This figure is also representative of the results at other times. It is seen in Figure 3-2 that below 400 km altitude $\sum_{i=0}^{6} \epsilon_i$ is comparable to or greater than the number densities of each of the deviations for all 6 energy levels. Above 400 km $\sum_{i=0}^{6} \epsilon_i$ is only several tens of percent of the deviations for levels 2 through 5 and a few percent of the deviations for levels 0 and 1. It should be pointed out that at 160 km, the ratio of the magnitudes of the deviations of level zero to level five (that is $\epsilon_0 / \epsilon_5$) is $10^7$ initially, and for the time corresponding to Figure 3-2, is near $10^6$. This explains why the ratios at 160 km increase with level number. At 840 km, altitude, for the time corresponding to Figure 3-2, the ratio of $\epsilon_0 / \epsilon_5$ is near $10^2$. It is significant that the ratio $\left| \sum_{i=0}^{6} \epsilon_i / \epsilon_i \right|$ has its largest values at the lowest altitudes where the deviations $\epsilon_i$ are numerically the largest. At low altitudes $\sum_{i=0}^{6} \epsilon_i$ is about $10^{-4}$ of the molecular nitrogen number density and at high altitudes it is about $10^{-3}$ of the molecular nitrogen number density. Figure 3-2 indicates that caution should be exercised in using the calculated deviations, $\epsilon_i$, only for altitudes below 370 km. However, as later sections show, the influence of the deviations below 370 km altitude is not large, but the $\epsilon_i$ do become physically important at higher altitudes where the precision of determination is considerably improved.

3.1 Solution for the Boltzmann part.

The vibrational temperatures calculated from the solution of the $\psi$ equation are shown versus altitude and time in Figures 3-3 and 3-4, respectively. The solutions are for the set 2 (initial and lower boundary vibrational temperature of 355°K) boundary conditions.
Figure 3-2. $\sum_{i=0}^{5} \frac{\varepsilon_i}{\varepsilon_i}$ for energy levels 0 through 5
Figure 3–3 shows the vibrational temperature profiles, calculated at five time steps, versus altitude. It is seen from this figure that at altitudes above 600 km the vibrational temperature is nearly isothermal at each time step, a result of the rapidity of the diffusion process at these altitudes. The downward movement of the energy is apparent in the figure. Vertical vibrational temperature gradients of as much as 25°C/km. are observed in the steady state.

Figure 3–4 is a plot of vibrational temperature versus time at ten altitudes of interest. It is seen from the figure that a steady state is reached in about one day. However, in 10 hours, or less depending on altitude, the vibrational temperature has achieved 90% or more of the steady state value. Notice that the vibrational temperature at the higher altitudes has a very steep gradient with time, initially. This rapid heating rate is important to the solutions of the deviation equations discussed in the next section. It should be noticed that the temperature at 240 km altitude has reached 1350°C, a value large enough to significantly affect the reaction constant of reaction (1–1), as discussed in section 3.3.

3.2 Solutions for the deviation parts.

It was found that convergence of the deviation solutions could not be achieved, even with 1 second time steps, if the solution was started at the "turn on" of the SAR-arc. It was determined that the difficulty was caused by terms involving derivatives of ψ and was apparently due to the initially very large changes in ψ primarily, those with time. Convergence of the solutions of the φ1 equations was obtained if the solutions were started at 5200 seconds "into" the arc, and this was the approach adopted. The physical conditions corresponding to the initial stages of a SAR-arc are unknown. However, it is expected that the characteristic times
Figure 3-3. Vibrational temperatures calculated from the ψ equation solutions versus altitude for five time steps.
Figure 3-4. Vibrational temperatures calculated from the $\psi$ equation versus time for several altitudes
of the important processes are measured in terms of one or more hours. Thus, the imposition of SAR-arc conditions in a step-wise manner is not realistic; so that little physical content has been lost by the adopted calculational approach.

Figures 3-5 through 3-10 show the φ_i's versus altitude for three time steps. These figures show that above 500 km the ratio of the deviation from the Boltzmann solution to the Boltzmann population, at the energy level of interest, is nearly constant with altitude. This result is again due to the rapidity of the diffusion process at these altitudes. It is also apparent from these figures that at altitudes of 300 km and above the φ_i's rapidly reach a maximum and then decrease to their "steady state" values. In these figures, where φ_i changes sign with altitude the absolute value has been plotted. It is seen that the "steady state" deviation populations above 300 km altitude, are less than the Boltzmann population of the corresponding energy levels 0, 1, 2 and 3 and are greater than the Boltzmann population for levels 4 and 5. This will be important in the calculation of an effective reaction coefficient for reaction (1-1) (see section 3.3).

Figures 3-11 through 3-16 show the φ_i's versus times for several altitudes. From these figures it is seen that above 300 km altitude a nearly constant, significant, deviation is maintained from a Boltzmann distributed population for the upper energy levels.

3.3 Reaction rate constant for reaction (1-1) and ionospheric loss time constant.

The effective reaction rate constant for the ion-atom interchange reaction (1-1) was calculated from
Figure 3-5. $|\varphi_0|$ versus altitude for 3 time steps
Figure 3-6. $|\varphi_1|$ versus altitude for 3 time steps
Figure 3-7. $|\varphi_2|$ versus altitude for 3 time steps
Figure 3-8. $|\phi_3|$ versus altitude for 3 time steps
Figure 3-10. $\phi_5$ versus altitude for 3 time steps
Figure 3-11. $|\phi_0|$ versus time for several altitudes
Figure 3-12: $|\phi_1|$ versus time for several altitudes
Figure 3-13. $|\phi_2|$ versus time for several altitudes
Figure 3-14. $|\phi_3|$ versus time for several altitudes
Figure 3-15. $\phi_4$ versus time for several altitudes
Figure 3-16. $\phi_5$ versus time for several altitudes.
Figure 3-17. Ratio of the effective to the energetically equivalent reaction constant, $k_e/k_B$, versus time for several altitudes.
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\[ k_e = \sum_{i=0}^{n} k(i) \frac{n_i}{n} \]

\[ = \sum_{i=0}^{n} k(i) \frac{(n'_i + \epsilon_i)}{n} \]  

(3-1)

where \( k_e \) is the effective rate constant and \( k(i) \) is the rate constant for level \( i \), taken from reference (13) and listed in Table 3. The reaction rate for the Boltzmann part of the solution, \( k_B \), was calculated from equation (3-1) with the \( \epsilon_i \) terms set to zero. The computer program for these calculations, REACTRAT, is listed in Appendix III.

A comparison of \( k_e \) and \( k_B \) is a measure of the importance of the deviation from a Boltzmann distribution to the \( F_2 \) region ionospheric ionization loss.

Figure 3-17 shows the ratio \( k_e/k_B \) versus time for several altitudes of interest. It is apparent in the figure, that for altitudes above 320 km the ratio is significantly larger than 1 throughout the time interval of the solutions, and particularly during the first 10 hours, the approximate duration of SAR-arcs.

Figure 3-18 shows the ratio \( k_e/k_B \) versus altitude for five time steps. It is seen in the figure that for a given time step the ratio is relatively constant with altitude for altitudes above 500 km. There is a large variation of the ratio with altitude between 280 km and 500 km, the region of the atmosphere where diffusion becomes the dominant process. This figure shows that the deviations from a Boltzmann solution are noticeable for altitudes as low as 300 km.

Figures 3-19 and 3-20 show the effective rate constant, calculated from equation 3-1 using the \( \psi \) and \( \phi_i \) equation solutions, versus time and altitude, respectively. These figures show that the rate constant can be factors of 2 to 8 times larger than
Figure 3-18. Ratio of the effective to the energetically equivalent reaction constant, $k_e/k_B$, versus altitude for five time steps.
Figure 3-19. Effective reaction rate constant versus time for several altitudes
Figure 3-20. Effective reaction rate constant versus altitude for five time steps
the value for vibrational temperatures near 300°K (shown as a triangle in the two figures).

The $k_e$ values, shown in Figures 3-19 and 3-20, have been used to calculate the loss rate for the ionospheric electrons and the ionospheric 'loss time constant' in the following way. Assuming reaction (1-2) is infinitely fast, then the electron loss rate will be the same as the $O^+$ ion loss rate. Further assuming the electron density and the $O^+$ ion density are the same, we have

$$\frac{d n_e}{dt} = -k_e n n_e$$

where $n_e$ is the electron density. The loss rate for the electrons is defined from (3-2) to be

$$\frac{1}{\tau} = k_e n$$

where $\tau$ is the ionospheric loss time constant.

Figure 3-21 and 3-22 show the loss time constant calculated from (3-3) versus altitude and time respectively. In Figure 3-21 the loss rate for four time steps and the 'normal' (vibrational temperature of 300°K) ionospheric time constant are shown. Noticeable decreases in the ionospheric loss time constant from the 'normal' value is observed at altitudes as low as 280 km.

Figure 3-22 shows the loss time constant versus time for several altitudes where the time constant is one day or less. It is seen from the figure that in the first 10 hours, the time constant at 360 km. altitude, where the 'normal' value is approximately 90 minutes, decreases to a value of 30 minutes. This figure shows
Figure 3-21. Ionospheric loss time constant versus altitude for four time steps
Figure 3-22. Ionospheric loss time constant versus time for altitudes where the time constant is 24 hours or less.
that the ionospheric loss time constant is decreased by factors larger than three in altitude regions between 360 km and 440 km where the ionospheric loss time constant is measured in hours.

3.4 The effects of: neglect of $\epsilon_j/n$; boundary conditions; and atomic oxygen loss process.

To determine the effect of the approximation of neglecting the $\epsilon_j/n$ term in the right hand side of the $\psi$ equation, (A2-30), the solutions of the $\phi_i$ equations were used to calculate the $\epsilon_j/n$ terms. Equation (A2-30) was then solved using those $\epsilon_j/n$ terms. The second approximation to $\psi$ was then used to recalculate the $\phi_i$'s.

The second approximation to $\psi$ yielded a vibrational temperature which was different from that obtained from the first approximation by 67 K, or less, at higher altitudes. At lower altitudes the difference was only a few degrees. The $\sum_{i=0}^1 \epsilon_i$ terms from the new solutions were also reduced by as much as a factor of 3. Thus, as expected on the basis of the $\sum_{i=0}^1 \epsilon_i$ results from the first solution, the second approximation to $\psi$ produces only a few percent correction to the results of the first approximation. The $\epsilon_i$'s calculated from the second approximation differed from those of the first approximation by 30%, or less, with most of the difference occurring at altitudes below 360 km. The $\sum_{i=0}^1 \epsilon_i$ term changed by a few tens of percent only. It is concluded, that the second approximation produces a negligible correction to the $\psi$ equation. Because most of the influence of the $\epsilon_i$'s is at altitudes above 300 km. (see section 3.3), the second approximation to the $\epsilon_i$'s is different from the first by only several percent in its impact on the ionospheric electron loss rates, and is therefore also negligible.
The $\psi$ and $\phi_i$ equations were resolved using set 1 boundary conditions. It was found that the vibrational temperature calculated from the $\psi$ equation solution differed from that obtained using set 2 boundary conditions by only a few degrees. The $\epsilon_i$ results differed by less than 3%. These results indicate that the solutions are not sensitive to the details of the loss mechanisms at the lower boundary.

An interesting result was obtained by comparing the behavior of the solutions with and without inclusion of the atomic oxygen production and loss processes for vibrational excitation, for set 1 boundary conditions (that is $T_v(120, t) = T_v(z, 0) = 0^\circ K$). The solution including the oxygen process yielded vibrational temperatures that were larger at all altitudes than those obtained from solutions not including the atomic oxygen processes. The largest differences between the two solutions initially occurred at altitudes below 320 km and was greater than 150$^\circ$K. This location for the differences is expected because this is the altitude region where the oxygen effects are relatively the most important. This result can be explained by the fact that the boundary condition of 0$^\circ$K vibrational temperature causes the initial vibrational temperatures to be less than the gas temperature, thus the atomic oxygen is a source of vibrational excitation through translational-vibrational energy exchange. Eventually the electronic source of vibrational energy dominates the solution. In the "steady state" the vibrational temperature corresponding to the solution with no atomic oxygen processes has a vibrational temperature only 8$^\circ$K greater at 160 km altitude and 6$^\circ$K greater at 920 km altitude than that corresponding to the solution containing the atomic oxygen processes.

A comparison of the $\phi_i$ equation solutions for these two cases is complex. At altitudes below 280 km, the $\epsilon_i$ initially changed by factors as large as 30 and 40
with the largest values of $\epsilon_i$ corresponding to the solutions containing the oxygen processes. Above 320 km altitude the two solutions for the $\epsilon_i$'s differ by approximately 25% or less. The $\epsilon_i$'s of the upper two energy levels show the smallest differences between the two solutions. The two sets of solutions for the $\epsilon_i$'s approach the same values in the steady state. The influence of the differences in the two sets of solutions on the ionospheric loss rates is small because the large differences occur below 320 km altitude where the deviations from the Boltzmann part of the solutions play a small part in the determination of the reaction rate constant.
CHAPTER IV. SUMMARY AND CONCLUSIONS

The objective of this work was to determine if the observed decrease in ionospheric electron density occurring in SAR-arcs could be explained by an increase in the reaction constant for the rate determining ion-atom interchange reaction (1-1). The increase in the reaction constant is due to vibrational excitation of molecular nitrogen by subexcitation, inelastic collisions between ambient, thermal, electrons and nitrogen molecules. The finding of this work is that the vibrational excitation of molecular nitrogen is indeed important to the ionosphere under SAR-arc conditions and can cause the loss time constant for the $F_2$ region to change to lower values by factors of 1.6 to 5 with an attendant decrease in the electron density.

Previous work, (20), (22) on the related problem of the diurnal variation of the molecular nitrogen vibrational temperature assumed the vibrational distribution to be Boltzmann and considered diffusion processes. Earlier work (23) in the vertical distribution of vibrationally excited molecular nitrogen in aurora ignored diffusion and solved the continuity equations for the excited energy levels of molecular nitrogen. This work solves the continuity equations for the first six energy levels of molecular nitrogen including the diffusion process. Thus, it combines into one solution, the previous approaches.

The continuity equations to be solved are six, coupled, mildly non-linear, partial differential equations containing the dominant source and loss terms for vibrational excitation of molecular nitrogen. The solutions were divided into an energetically equivalent part that is Boltzmann distributed and a part representing deviations from the Boltzmann solution. The resulting equations were solved...
numerically, using finite difference equations, to provide the populations of the
energy levels as functions of time and altitude.

It was found, under conditions where the ionospheric electron temperature
reaches values near 5000°K at 500 km altitude, that the vibrational temperature
of molecular nitrogen reached a steady state value near 2300°K. at that altitude.
The deviations from the Boltzmann distribution depends strongly on altitude for
altitudes below 400 km. This is the region of the atmosphere where the diffusion
process becomes dominant with increasing altitude over the vibrational-vibrational
energy exchange process. It was found that for the highest three energy levels,
above 300 km. altitude, the deviations from a Boltzmann distribution increased
the populations of these levels by factors of 2 to 10. These results were insensi-
tive to plausible variations of the boundary conditions.

The deviations from a Boltzmann distribution caused the effective reaction
rate for reaction (1-1) to be increased by as much as a factor of 1.7 over the value
obtained from the energetically equivalent Boltzmann solution. This indicates the
possible importance of these deviations in problems involving chemical reactions
at altitudes as low as 500 km. The effective reaction rate, calculated using the
total population densities, was as much as a factor of 8 greater than the reaction
rate for a vibrational temperature of 300°K. Significant enhancements of the re-
action rate were found to occur at altitudes as low as 300 km.

Because of these increased reaction rates, the times required to significantly
decrease the electron density in the ionosphere were reduced from their normal
value by factors of 1.6 to 5, depending on altitude. Over most of the altitude range
where the loss time is short compared to SAR-arc durations, the loss time was
reduced by factors exceeding 1.8.

These results lead to the conclusions that the vibrational excitation of molec-
ular nitrogen, under conditions corresponding to SAR-arcs, causes a large increase
in the loss rate of ionospheric electrons in the $F_2$ region. The enhanced loss rate
is of such magnitude, that it alone will account for the observed electron density
depressions in SAR-arcs.
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<td>$\sigma_{54}$</td>
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TABLE 2

Parameters for Reaction Rate Constants for Production and Loss of Vibrational Excitation by Electron Collisions

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### TABLE 3

**Reaction Rates for Vibrational Levels**

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</tr>
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<td>11</td>
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APPENDIX I

ELECTRONIC PRODUCTION AND LOSS OF VIBRATIONAL EXCITATION

Production and loss rates for the first six vibrational levels of molecular nitrogen were calculated using theoretically calculated (28), (29), (30) cross-sections for inelastic, sub-excitation, electron scattering for these levels. The cross-sections were averaged over the Maxwell-Boltzmann energy distribution representing the electron gas to produce the production and loss rates. This section contains an amplified outline of the content of the theoretical cross-section calculations in Chen's, (28), (29) papers as well as discussion of the calculation of reaction rates.

Chen (28), (29) applies the unified theory of Feshbach (37), for nuclear reactions involving the formation of a compound state, to inelastic scattering of electrons by molecules. Hereafter Chen (28) will be called paper I and equations contained therein referenced as I X.XX. Chen (29) will be referenced as paper II and equations contained therein will be referenced as II X.XX.

A1.1 Paper I:

Paper I starts with the consideration of an N-electron system consisting of an incident electron and a diatomic target molecule with N-1 electrons. The system is separated into relative and center of mass coordinates and the center of mass part is removed from the Schrodinger equation. The relative coordinates for the electrons, $\vec{X}$, $\vec{r}_1$, $\vec{r}_2$, ..., $\vec{r}_{N-1}$, are referenced to the center of mass of the nuclei. $X$ refers to the incident electron. $\vec{R}$ is the vector separation of the two heavy nuclei a and b with masses $M_a$ and $M_b$ respectively. The Schrodinger
equation is (in atomic units)

\[
[K_0(\vec{X}) + V_0(\vec{X}, \vec{r}, \vec{R}) + H_{ab}(\vec{r}, \vec{R})] \Omega = E\Omega
\]  \hspace{1cm} (I2.1)

where

\[
V_0(\vec{x}, \vec{r}, \vec{R}) = \sum_{i=1}^{N-1} \frac{1}{|\vec{x} - \vec{r}_i|} - \frac{Z_a}{X_a} - \frac{Z_b}{X_b}
\]  \hspace{1cm} (I-2.2)

and \(\vec{r}\) is the collective notation of \(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_{N-1}\) for the molecular electrons; \(K_0\) is the kinetic energy operator of the incident electron; \(V_0\) is the Coulombic potential energy of the incident electron; \(H_{ab}\) is the Hamiltonian for the target molecule; \(\Omega\) is the total wavefunction for the system having the total energy \(E\); \(X_a\) and \(X_b\) are the position vectors of the incident electron with respect to the two nuclei having \(Z_a\) and \(Z_b\) as their charges.

It is assumed that the unperturbed molecule is described by the set of Schrödinger equations

\[
H_{eI}(\vec{r}, \vec{R}) \Phi_e(\vec{r}, \vec{R}) = \epsilon_e(\vec{R}) \Phi_e(\vec{r}, \vec{R})
\]  \hspace{1cm} (I-2.3)

\[
[-(2\mu)^{-1} \nabla^2_R + \epsilon_e(\vec{R})] \chi_{e\gamma}(\vec{R}) = \epsilon_{e\gamma} \chi_{e\gamma}(\vec{R})
\]  \hspace{1cm} (I-2.4)

where

\[
H_{eI}(\vec{r}, \vec{R}) = \frac{1 + M_a + M_b}{2 (M_a + M_b)} \sum_{i=1}^{N-1} \nabla_i^2 + U_{eI}(\vec{r}, \vec{R})
\]  \hspace{1cm} (I-2.5)

and

\[
\mu = \frac{M_a M_b}{M_a + M_b}; \quad \nabla_i^2
\]

is the Laplacian operator on coordinate \(i\) and \(U_{eI}\) is the potential energy of the molecular electrons.
The cross terms for electrons and electron-nuclei contained in the Born-Oppenheimer separation are neglected because they do not enter, in the zeroth order approximation, in the expression for the excitation of nuclear motion, (34), pages 925-928. The electronic wavefunctions, \( \phi_n \), and nuclear wavefunctions \( \chi_{n\gamma} \) having eigenvalues \( \varepsilon_n (R) \) and \( \varepsilon_{n\gamma} \), respectively, form a complete, orthogonal set in their corresponding spaces.

The total wavefunction is expanded in terms of \( \phi_n \) and \( \chi_{n\gamma} \) to give

\[
\Omega(X, \vec{r}, \vec{R}) = \sum_{n, \gamma} \Phi_n(\vec{r}, \vec{R}) \chi_{n\gamma}(\vec{R}) \psi_{n\gamma}(\vec{X})
\]

where exchange effects are neglected. The expansion coefficients \( \psi_{n\gamma}(\vec{x}) \) are assumed not to depend on the inter-nuclear separation as a parameter. It is assumed that the inter-nuclear separation is fixed at its equilibrium value \( R_e^{(0)} \) for \( \psi_{n\gamma}(\vec{X}) \). The effect of this assumption is estimated to be of order \( \mu^{-1} \).

Substituting equation (I-2.7) into the Schrödinger equation (I-2.1), multiplying on the left by \( \Phi_{n'}^* \), \( \chi_{n', \gamma'}^* \), integrating over \( \vec{r} \) and \( \vec{R} \) and using (I-2.3) through (I-2.6) we have the coupled sets of equations

\[
[K_0(\vec{X}) + \varepsilon_{n\gamma} - E] \psi_{n\gamma}(\vec{X}) = \sum_{n', \gamma'} V_{n'n'}^{\gamma\gamma'}(\vec{X}) \psi_{n', \gamma'}(\vec{X})
\]

with

\[
V_{n'n'}^{\gamma\gamma'}(\vec{x}) = \langle \chi_{n'\gamma'} | V_{n'n'}(\vec{x}, \vec{R}) - (2\mu)^{-1} C_{n'n'}(R, \nabla_R) | \chi_{n'\gamma'} \rangle
\]

\[
V_{n'n'}(\vec{X}, \vec{R}) = \langle \phi_n | V_0(\vec{X}, \vec{R}, \vec{r}) | \phi_{n'} \rangle
\]
\[ C_{nn'} = 2 \left\langle \Phi_n | \nabla R | \Phi_{n'} \right\rangle \cdot \nabla R + \left\langle \Phi_n | \nabla^2 R | \Phi_{n'} \right\rangle \]  \hspace{1cm} (I-2.11)

Because we are interested in subexcitation electron impact, the \( \psi_{0\gamma} \)'s are of particular interest. Thus writing (I-2.8) as

\[
[K_{0}(\bar{X}) + \epsilon_{0\gamma} - E] \psi_{0\gamma}(\bar{X}) = - \sum_{\gamma'} V_{00}^{\gamma\gamma'} \psi_{0\gamma'}(\bar{X}) - \sum_{n', \gamma', n' \neq 0} \psi_{n', \sigma}(\bar{X}) \tag{A1-1}
\]

and

\[
[K_{0}(\bar{X}) + \epsilon_{n\gamma} - E] \psi_{n\gamma}(\bar{X}) = - \sum_{\gamma'} V_{nn}^{\gamma\gamma'} \psi_{n\gamma'}(\bar{X}) - \sum_{n', \gamma', n' \neq 0} V_{n'n}^{\gamma\gamma'} \psi_{n', \gamma'}(\bar{X}) \tag{A1-2}
\]

for \( n \neq 0 \).

Rewriting (1) and (2) we have

\[
[K_{0}(\bar{X}) + \epsilon_{0\gamma}] \psi_{0\gamma}(\bar{X}) + \sum_{\gamma'} V_{00}^{\gamma\gamma'} \psi_{0\gamma'}(\bar{X}) - E\psi_{0\gamma}(\bar{X}) = - \sum_{n', \gamma', n' \neq 0} V_{0n}^{\gamma\gamma'} \psi_{n', \gamma'}(\bar{X}) \tag{A1-3}
\]

\[
[K_{0}(\bar{X}) + \epsilon_{n\gamma}] \psi_{n\gamma}(\bar{X}) + \sum_{n', \gamma', n' \neq 0} V_{nn}^{\gamma\gamma'} \psi_{n', \gamma'}(\bar{X}) - E\psi_{n\gamma}(\bar{X}) = - \sum_{\gamma'} V_{n0}^{\gamma\gamma'} \psi_{0\gamma'}(\bar{X}) \tag{A1-4}
\]

Defining

\[
T_n = \begin{bmatrix}
K_0 + \epsilon_{n0} \\
K_0 + \epsilon_{n1} & 0 \\
K_0 + \epsilon_{n2} & 0
\end{bmatrix} \tag{I-2.14}
\]
\[ \psi_n = \begin{bmatrix} \psi_{n0} \\ \psi_{n1} \\ \vdots \\ \psi_{n2} \\ \vdots \end{bmatrix} \] (I-2.12)

\[ \psi = \begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \end{bmatrix} \] (I-2.15)

\[ U_{nn'} = \begin{bmatrix} V_{nn'}^{00} & V_{nn'}^{01} & V_{nn'}^{02} & \cdots \\ V_{nn'}^{10} & V_{nn'}^{11} & V_{nn'}^{12} & \cdots \\ V_{nn'}^{20} & V_{nn'}^{21} & V_{nn'}^{22} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \] (I-2.13)

\[ U_0 = (U_{01}, U_{02}, U_{03}, \ldots) \] (I-2.16)

\[ U'_0 = \begin{bmatrix} U_{10} \\ U_{20} \\ U_{30} \\ \vdots \end{bmatrix} \] (I-2.17)
(3) and (4) become

\[ T_0 \psi_0 + U_{00} \psi_0 - E \psi_0 = - \sum_{n' \neq 0} U_{0n'}, \psi_n' = - U_0 \psi \]  \hspace{1cm} (I-2.19)

and

\[ T_n \psi_n + \sum_{n' \neq 0} U_{nn'}, \psi_n' - E \psi_n = - U_{n0} \psi_0 \]

or

\[ (H - E) \psi = - U_0' \psi_0 \]  \hspace{1cm} (I-2.20)

where

\[
H = \begin{bmatrix}
T_1 + U_{11} & U_{12} & U_{13} & \cdots \\
U_{21} & T_2 + U_{22} & U_{23} & \cdots \\
U_{31} & U_{32} & T_3 + U_{33} & \cdots \\
& \ddots & \ddots & \ddots \\
& & & \ddots & \ddots & \ddots
\end{bmatrix}
\]  \hspace{1cm} (I-2.18)

and

\[ E_{nn'} = E \delta_{nn'}, \]

Following Fishbach's formalism, (37), the formal solution of (I-2.20) is

\[ \psi = (E - H + i \eta)^{-1} U_0' \psi_0 \]  \hspace{1cm} (I-2.21)

where \( \eta = \eta \delta_{ij} \) and \( \eta \rightarrow 0^+ \) to ensure outgoing waves in the exit channels, (I-2.21) gives \( \psi \) in terms of \( \psi_0 \). Using (I-2.21) in (I-2.19), we obtain

\[ (T_0 + \Lambda - E) \psi_0 = 0 \]  \hspace{1cm} (I-2.22)
where

\[ \Lambda = U_{00} + U_0 (E - H + i \eta)^{-1} U'_0 \]  

(I-2.23)

and is the effective scattering potential for subexcitation scattering of electrons by molecules.

The formal solution (I-2.21) contains the Green's function operator \( \lim_{n \to 0^+} (E_1 - H + i \eta)^{-1} \) which implies the need for a set of eigenfunctions of the effective Hamiltonian \( H \). Thus we write

\[ H \Psi_m = W_m \Psi_m \]  

(I-3.2)

where a set of eigenfunctions \( \{ \Psi_m \} \) approximates the set of compound negative ion eigenfunctions with energy spectrum \( \{ W_m \} \).

The physical significance of these states is illustrated in the weak coupling limit where \( H \) is diagonal. In this case (I-3.2) gives the equations

\[ (T_n + U_{nn}) \psi^{(m)}_n = W^{(m)}_n \psi^{(m)}_n \quad n \neq 0 \]  

(I-3.3)

which is expanded further to become

\[ [K_0 + V_{nn} + \epsilon_{n0} - W_{n\gamma}] \psi^{(m)}_n = - \sum_{\gamma' \neq \gamma} V_{n\gamma}^{\gamma'\gamma} \psi^{(m)}_{n\gamma'} \]  

(I-3.4)

The compound negative ion states \( \psi^{(m)}_n \) describe, in this instance, a set of states of the incident electron in resonance with the field of the excited target molecule.

Expanding the Green's function operator contained in (I-2.21) in terms of the eigenfunctions \( \Psi_m \) we have
\[ G^{(+)}(E) = \sum_{m} \frac{|\Psi_{m}^{+} \langle \Psi_{m}^{-} |}{E - W_{m}} + \int d\rho \int dW \frac{|\Psi(\rho, W) \langle \Psi(\rho, W)|}{E - W + i\gamma} \quad (I-4.1) \]

where the sum over \( m \) is for the discrete states and the integral over \( \rho \) contains the continuous eigenspectrum for energy \( E \). Expression \( (I-4.1) \) implies a resonance part of the operator and a non-resonance part. Therefore we write

\[ G^{(+)}(E) = Q(E) + G_{0}^{(+)}(E) \quad (I-4.2) \]

with

\[ Q(E) = \sum_{m} \frac{|\Psi_{m}^{+} \langle \Psi_{m}^{-} |}{E - W_{m}} \quad (I-4.3) \]

\( Q(E) \) is the resonance part of the operator and the prime means that only those negative ion states having energies comparable to that of the system are included in the summation. The effective potential \( (I-2.23) \) is now written, using \( (I-4.2) \) in \( (I-2.23) \) as

\[ \Lambda = u' + u \quad (I-4.4) \]

where

\[ u' = U_{0} Q(E) U_{0}' \quad (I-4.5) \]

\[ u = U_{00} + U_{0} G_{0}^{(+)}(E) U_{0}' \quad (I-4.6) \]

Let \( \pi_{0}^{(-)} \) be the solution for an outgoing wave of the equation

\[ (T_{0} - E) \pi_{0}^{(-)} = 0 \]
Using (I-4.4) in (I.22) we have

\[(T_0 + U - E) \psi_0 = -u' \psi_0 \quad \text{(A1-5)}\]

where the resonance part of the effective scattering potential is treated as the scattering potential.

From scattering theory, (38), Chapter 12, the solution for the outgoing wave is

\[\psi_0 = \psi_0^{(+)} + (E - T_0 - u + i \eta)^{-1} u' \psi_0 \quad \text{(I-4.12)}\]

where

\[(T_0 + u - E) \psi_0^{(+)} = 0 \quad \text{(I-4.10)}\]

and \(\psi_0^{(+)}\) is an incoming wave and contains the effects of the direct scattering potential \(u\).

The transition matrix describing transitions from the incident channel \(\gamma'\) to channel \(\gamma\) for \(n = 0\) is

\[\mathcal{J}_0(\gamma, \gamma') = \langle \pi_0^{(-)}(\gamma) | u + u' | \psi_0(\gamma') \rangle \quad \text{(I-4.13)}\]

Consider the outgoing wave solutions to

\[(T_0 + u - E) \psi_0^{(-)} = 0 \quad \text{(A1-6)}\]

which may be written as

\[\psi_0^{(-)} = \pi_0^{(-)} + (E - T_0 - i \eta)^{-1} u \psi_0^{(-)} \quad \text{(I-4.14)}\]
Multiplying by \((E - T_0 - i \eta)\) and adding and subtracting \(u \pi_0^{(-)}\) to the right hand side we have

\[
(E - T_0 - i \eta) \psi_0^{(-)} = (E - T_0 - i \eta) \pi_0^{(-)} + u \psi_0^{(-)} + u \pi_0^{(-)} - u \pi_0^{(-)} \quad (A1-7)
\]

\[
\therefore \psi_0^{(-)} = \pi_0^{(-)} + (E - T_0 - u - i \eta)^{-1} u \pi_0^{(-)} \quad (I-4.15)
\]

\[
\therefore \pi_0^{(-)} = \psi_0^{(-)} - (E - T_0 - u - i \eta) u \pi_0^{(-)} \quad (A1-8)
\]

Substituting \((A-1-8)\) in \((I-4.13)\) we have

\[
\mathcal{G}_0(\gamma, \gamma') = \langle \pi_0^{(-)} | u | \psi_0 \rangle - \langle (E - T_0 - u - i \eta)^{-1} u \pi_0^{(-)} | u' | \psi_0 \rangle \\
+ \langle \psi_0^{(-)} | u' | \psi_0 \rangle \\
= \langle \pi_0^{(-)} | u | \psi_0 \rangle - (E - T_0 - u + i \eta)^{-1} u' \psi_0 \\
+ \langle \psi_0^{(-)} | u' | \psi_0 \rangle \\
= \langle \pi_0^{(-)} | u | \psi_0^{(+)} \rangle + \langle \psi_0^{(-)} | u' | \psi_0 \rangle \quad (A1-9)
\]

using \((I-4.12)\). Consider \(\langle \psi_0^{(-)} | u' | \psi_0 \rangle\) and repeatedly substitute \((I-4.12)\) for \(\psi_0\) to obtain

\[
\langle \psi_0^{(-)} | u' | \psi_0 \rangle = \langle \psi_0^{(-)} | u' | \psi_0^{(+)} \rangle + \langle \psi_0^{(-)} | u' (E - T_0 - u + i \eta)^{-1} u' | \psi_0 \rangle \\
= \langle \psi_0^{(-)} | u' | \psi_0^{(+)} \rangle + \langle \psi_0^{(-)} | u' (E - T_0 - u + i \eta)^{-1} u' | \psi_0^{(+)} \rangle \\
+ \langle \psi_0^{(-)} | u' (E - T_0 - u + i \eta)^{-1} u (E - T_0 - u + i \eta)^{-1} u' | \psi_0^{(+)} \rangle \\
+ \cdots \\
= \langle \psi_0^{(-)} | u' + u' (E - T_0 - u + i \eta)^{-1} u' + u' (E - T_0 - u + i \eta)^{-1} u' \cdot (E - T_0 - u + i \eta)^{-1} u' + \cdots | \psi_0^{(+)} \rangle \quad (A1-10)
\]
For an isolated resonance, the summation over \( m \) in (I-4.3) reduces to one term
and (I-4.5) becomes

\[
u' = \frac{U_0 |\Psi_m\rangle \langle \Psi_m | U'_0}{E - W_m}
\]  

(A1-11)

Thus (11) becomes

\[
\langle \psi_0^- | u' | \psi_0^+ \rangle = \frac{\langle \psi_0^- | U_0 | \Psi_m \rangle \langle \Psi_m | U'_0 | \psi_0^+ \rangle}{E - W_m}
\]

\[
\left\{ 1 + \frac{\langle \Psi_m | U'_0 (E - T_0 - u + i \eta)^{-1} U_0 | \Psi_m \rangle}{E - W_m} + \cdots \right\}
\]

Let

\[
R_m = \langle \Psi_m | U'_0 (E - T_0 - u + i \eta)^{-1} U_0 | \Psi_m \rangle 
\]  

(I-4.23)

Therefore

\[
\langle \psi_0^- | u' | \psi_0^+ \rangle = \frac{\langle \psi_0^- | U_0 | \Psi_m \rangle \langle \Psi_m | U'_0 | \psi_0^+ \rangle}{E - W_m}
\]

\[
\left\{ 1 + \frac{R_m}{E - W_m} + \frac{R_m^2}{E - W_m} + \cdots \right\}
\]

\[
= \frac{\langle \psi_0^- | U_0 | \Psi_m \rangle \langle \Psi_m | U'_0 | \psi_0^+ \rangle}{E - W_m - R_m}
\]  

(I-4.24)

A1.2 Paper II.

In his application to molecular nitrogen, (29), Chen makes the following assumptions:

(1) an isolated resonance occurs.

(2) the direct transition amplitude is negligible.
(3) a single excited electronic state, \( n \), of the target molecule is responsible for the resonance.

(4) the nuclear states of the target molecule are not strongly coupled and the Born–Oppenheimer coupling matrix elements are negligible.

(5) the total contribution to the transition amplitudes due to resonance effects of the set of compound negative-ion states may be accounted for as a linear sum of the individual contribution of each compound state.

From assumptions (1) and (2) equation (I-4.24) gives the transition matrix element. Thus

\[ G_0(\gamma, \gamma') = \frac{\langle \psi_0^- | U_0 | \Psi_m \rangle \langle \Psi_m | U_m' | \psi_0^+ \rangle}{E - W_m - R_m} \]  

(II-2.2)

From assumption (3) only \( V_{on} \), \( V_{no} \), \( V_{nn} \) and \( V_{oo} \) in equation (I-2.10) are non-zero. Thus \( H \) in equation (I-2.18) becomes a single element matrix. Assumption (4) gives from equations (I-2.11) and (I-2.9) respectively

\[ C_{nn'} = 0 \quad \text{and} \quad V_{nn'} = 0. \]

Thus \( U_{nn} \) in equation (I-2.13) is diagonal. Therefore we have

\[ H \Psi_m = W_m \Psi_m \]

giving

\[ H_n \psi_n^{(m)} = W_n^{(m)} \psi_n^{(m)} \]

or

\[ (T_n + U_{nn}) \psi_n^{(m)} = W_n^{(m)} \psi_n^{(m)} \]  

(A1-12)
where

\[
\psi_{n}^{(m)}(\lambda) = \begin{bmatrix}
0 \\
0 \\
\vdots \\
\psi^{(m)}_{n\lambda} \\
0 \\
\vdots
\end{bmatrix}
\]

Expanding (A1-12) further and rearranging terms

\[
[K_0 + V_{nn}^{\lambda\lambda}] \psi_{n\lambda}^{(m)} = (W_{nn}^{(m)} - \epsilon_{n0}) \psi_{n\lambda}^{(m)}
\]

\[
= (\epsilon_{n\lambda} - \epsilon_{n}(R_{e}^{(m)})) \psi_{n\lambda}^{(m)}
\]

Now consider

\[
(U_0 | \psi_{m}^{(m)})_{\gamma} = \left( \sum_{r} U_{0r} \psi_{r}^{(m)} \right)_{\gamma}
\]

\[
= (U_{0n} \psi_{n}^{(m)})_{\gamma}
\]

\[
= V_{0n}^{\gamma\lambda} \psi_{n\lambda}^{(m)}
\]

Similarly

\[
(U_{0}^{*} | \psi_{m}^{(*)})_{\gamma} = V_{0n}^{\gamma'\lambda'} \psi_{n\lambda}^{(m)}
\]

The $\gamma' \rightarrow \gamma$ transition due to the $\lambda$ th vibrational level in the negative ion state is

\[
\delta_{\lambda}^{\lambda}(\gamma, \gamma') = \frac{\langle \psi_{0\gamma}^{(-)} | V_{0n}^{\gamma\lambda} | \psi_{n\lambda}^{(m)} \rangle \langle \psi_{n\lambda}^{(m)} | V_{n0}^{\gamma'\lambda'} | \psi_{0\gamma'}^{(+)} \rangle}{E - W_{n\lambda}^{(m)} + R_{n\lambda}^{(m)}}
\]
Using assumption (5), the total transition matrix element is

\[ \mathcal{G}_0(\gamma, \gamma') = \sum_\lambda \mathcal{G}_0^\lambda(\gamma, \gamma') \]

\[ = \sum_\lambda \frac{\langle \psi^{(-)}_0 | \mathbb{V}^{\gamma\lambda}_{0n} | \psi^{(m)}_n \rangle \langle \psi^{(m)}_n | \mathbb{V}^{\gamma'y'}_{n0} | \psi^{(+)}_{0y'} \rangle}{E - W^{(m)}_{n\lambda} + R^{(m)}_{n\lambda}} \]  

(II-2.3)

And

\[ R^{(m)}_{n\lambda} = \langle \psi^{(m)}_n | \sum_\gamma \mathbb{V}^{\gamma\lambda}_{0n} (E - H_0 + i\eta)^{-1} \mathbb{V}^{\gamma\lambda}_0 | \psi^{(m)}_n \rangle \]  

(II-2.5)

Expanding

\[ (E - H_0 + i\eta)^{-1} = \int dE_{\gamma} \frac{|\psi^{(+)}_{0\gamma} \rangle \langle \psi^{(-)}_{0\gamma}|}{E - E_{\gamma} + i\eta} \xi_{\gamma} \]

where \( \xi_{\gamma} \) is the density of states in the exit channel \( \gamma \), and using

\[ \frac{1}{E - E_{\gamma} + i\eta} = \frac{E - E_{\gamma}}{(E - E_{\gamma})^2 + \eta^2} - \frac{i\eta}{(E - E_{\gamma})^2 + \eta^2} \]

we have

\[ R^{(m)}_{n\lambda} = \Delta^{(m)}_{n\lambda} - i \frac{1}{2} \Gamma^{(m)}_{n\lambda} \]  

(II-2.5)

where

\[ \Delta^{(m)}_{n\lambda} = \langle \psi^{(m)}_n | \sum_\gamma \mathbb{P} \int \mathbb{V}^{\gamma\lambda}_{n0} \frac{E - E_{\gamma}}{(E - E_{\gamma})^2 + \eta^2} \langle \psi^{(+)}_{0\gamma} | \mathbb{V}^{\gamma\lambda}_{0n} \xi_{\gamma} dE_{\gamma} | \psi^{(m)}_n \rangle \]  

(II-2.8)
and

\[ \Gamma_{n\lambda}^{(m)} = 2 \delta m (R_{n\lambda}^{(m)}) \]

\[ = 2 \langle \psi_{n\lambda}^{(m)} \rangle \sum_{\gamma} \int V_{n\gamma}^{\lambda} \frac{\eta |\psi_{\gamma}^{(+)}\rangle \langle \psi_{\gamma}^{(-)}|}{(E - E_{\gamma})^2 + \eta^2} V_{\gamma n}^{\lambda} \xi_{\gamma} dE_{\gamma} | \psi_{n\lambda}^{(m)} \rangle \]  
(A1-15)

\[ = 2 \langle \psi_{n\lambda}^{(m)} \rangle \sum_{\gamma} \int V_{n\gamma}^{\lambda} |\psi_{\gamma}^{(+)}\rangle \langle \psi_{\gamma}^{(+)}\rangle |\psi_{\gamma}^{(-)}\rangle \langle \psi_{\gamma}^{(-)}| + \pi \delta (E - E_{\gamma}) V_{\gamma n}^{\lambda} \xi_{\gamma} dE_{\gamma} | \psi_{n\lambda}^{(m)} \rangle \]  
(A1-16)

Using

\[ \xi_{\gamma} = \frac{d\Omega_f}{(2\pi)^3} \frac{k_{\gamma} d(k_{\gamma}^2)}{dE_{\gamma}} \]

\[ = \frac{d\Omega_f}{(2\pi)^3} \frac{1}{2} \frac{k_{\gamma} d(k_{\gamma}^2)}{dE_{\gamma}} \]

and

\[ E_{\gamma} = \frac{1}{2} k_{\gamma}^2 \]

then

\[ \xi_{\gamma} = \frac{d\Omega_f}{(2\pi)^3} k_{\gamma} \]  
(A1-17)

Using (A1-17) to (A1-16) we have

\[ \Gamma_{n\lambda}^{(m)} = \frac{1}{(2\pi)^2} \sum_{\gamma} \int \langle \psi_{\gamma}^{(-)} \rangle \xi_{\gamma} V_{\gamma n}^{\lambda} \langle \psi_{n\lambda}^{(m)} \rangle^* | \psi_{n\lambda}^{(m)} \rangle |^2 k_{\gamma} d\Omega_f \]  
(II-2.9)

Using the definitions of \( V_{\gamma n}^{\lambda} \) and \( V_{n\gamma}^{\lambda} \) from equation (I-2.10) and interchanging the order of integration in (II-2.3) we obtain

\[ \Omega_0(\gamma, \gamma') = \sum_{\lambda} \frac{(X_{\gamma' \lambda} | X_{n\lambda} \rangle \langle X_{n\lambda} | \alpha_{\lambda \gamma'} \rangle | \alpha_{\lambda \gamma} \rangle^* | X_{\gamma' \lambda} \rangle}{E - E_{n\lambda}^{(m)} + i 1/2 \Gamma_{n\lambda}^{(m)}} \]  
(II-2.11)
and

\[ \Gamma^{(m)}_{n\lambda} = \sum_{\gamma} \frac{k_\gamma}{(2\pi)^2} \int |\langle \chi_{0\gamma} | \alpha_{\gamma\lambda} | \chi_{n\lambda} \rangle|^2 d\Omega_f \quad (\text{II}-2.12) \]

where

\[ \alpha_{\gamma\lambda} = \langle \psi_{0\gamma} | V_0 | \Phi_n \psi^{(m)}_{n\lambda} \rangle \quad (\text{II}-2.13a) \]

\[ \alpha^*_{\lambda\gamma} = \langle \psi_{n\lambda} | V_0 | \Phi_0 \psi^{(+)\dagger}_{0\lambda'} \rangle \quad (\text{II}-2.13b) \]

\[ E^{(m)}_{n\lambda} = W^{(m)}_{n\lambda} + \Delta^{(m)}_{n\lambda} = \epsilon^{(m)}_{n\lambda} + \Delta^{(m)}_{n\lambda} + \epsilon_{n\lambda} - \epsilon_n (R^{(n)}) \quad (\text{II}-2.14) \]

The differential partial cross section \( d\sigma_{\gamma'\gamma} \), is expressed as a function of the incident angles of the impinging electron by

\[ d\sigma_{\gamma'\gamma} = (4\pi^2)^{-1} \left| \mathcal{M}_{0}(\gamma, \gamma') \right|^2 d\Omega_f \]

where

\[ k_\gamma^2 = k_{\gamma'}^2 + 2(\epsilon_{0\gamma'} - \epsilon_{0\gamma}) \]

with the initial and final wavenumbers of the electron given by \( k_{\gamma'} \) and \( k_\gamma \) respectively.

Because the rotational motion of the molecule is relatively slow, the molecular orientation is considered fixed throughout the vibrational excitation or de-excitation. If the molecule remains in the ground rotational state then the partial cross-section can be obtained by averaging the transition matrix elements over the incident angles and integrating the resultant over the sphere of the final angles.

The result is

\[ \sigma_{\nu\nu'} = (16\pi^3)^{-1} \frac{k_\nu}{k_{\nu'}} \int \left| \mathcal{M}_{0}(\nu, \nu') \right|^2 d\Omega_0 d\Omega_f \quad (\text{II}-2.17) \]
where the $\gamma$'s have been replaced by $\nu$'s to reflect that the $\chi$'s now represent vibrational wave functions only.

The further assumption that the compound negative-ion state does not depend on the vibrational state is made. This assumption allows the cross-section to be written as

$$\sigma_{\nu\nu'} = \frac{\beta_\nu \beta_{\nu'} k_\nu k_{\nu'}}{16 \pi^3} \left| \sum_{\lambda} \frac{\alpha_{0\nu} \langle X_{n\lambda} | \chi_{n\lambda} | X_{0\nu'} \rangle}{E - E^{(m)}_{n\lambda} + i \frac{1}{2} \Gamma^{(m)}_{n\lambda}} \right|^2$$

(II-2.18)

with

$$\Gamma^{(m)}_{n\lambda} = \sum_{\nu} \beta_\nu k_\nu (2 \pi)^{-2} \left| \langle X_{0\nu} | \chi_{n\lambda} \rangle \right|^2$$

(II-2.19)

$$\beta_\nu = \int |a_{\nu 0}|^2 \, d\Omega_f$$

(II-2.20)

$$\beta'_{\nu} = \int |a_{0\nu'}|^2 \, d\Omega_0$$

(II-2.21)

$$E^{(m)}_{n\lambda} = \varepsilon_{n\lambda}^{(m)} + \Delta^{(m)}_{n0} + \varepsilon_{n\lambda} - \varepsilon_n (Re^n)$$

(II-2.22)

where the $\alpha$'s have been taken outside of the $R$ integrals because they vary slowly and most of their contribution comes from a narrow range of internuclear separation $R = Re^{(0)}$.

Chen used Morse anharmonic wavefunctions for the $\chi$'s and approximated the resonance energy (II-2.22) by

$$E^{(m)}_{n\lambda} = \varepsilon_{n0}^{(m)} + \Delta_{n0}^{(m)} + \left( \lambda + \frac{1}{2} \right) \omega^{(n)} - \left( \lambda + \frac{1}{2} \right)^2 \omega^{(n)} \chi_e^{(n)}$$

(II-3.3)
where $\omega_e^{(n)}/2$ is the zero point energy of the corresponding harmonic oscillator and the last term is an anharmonic correction. The $\beta$'s are found from the set of linear equations (II-2.19). The cross sections are then determined from (II-2.18).

The excited field for resonance was identified as the $x^1 \sum_g^-$ of N$_2$. Once the excited state is identified the energy scale and averaged peak widths are shifted and altered by varying two parameters $\epsilon^{(m)}_{n_0} + \Delta^{(m)}_{n_0}$ and $\Gamma^{(m)}_{n_0}$ until adjustment to the experimental data is achieved. The values giving the best fit are

$$\epsilon^{(m)}_{n_0} + \Delta^{(m)}_{n_0} = 1.89 \text{ ev}$$

$$\Gamma^{(m)}_{n_0} = 0.152 \text{ ev}$$

These values are then used in the calculation of the cross-sections for excitation and de-excitation for other levels. (See reference (30) for the corrected figures for reference (29).)

### A1.3 Calculation of reaction rates:

The reaction rate $I_{ij}$, is obtained from the cross section, $\sigma_{ij}$, by

$$I_{ij} = \int\int_{-\infty}^{\infty} v_e \sigma_{ij} (v_e) f (v_e) \, d^3 v_3 \quad (A1-18)$$

where

- $v_e$ is the electron velocity
- $f (v_e)$ is the distribution function for the electrons (assumed Maxwell-Boltzmann).

Equation (A1-18) when expressed in terms of electron energy, $E$ in eV, becomes
\[ I_{ij} = (1.26574 \times 10^{-6}) \pi \left( \frac{2}{\pi k T_e} \right)^{3/2} \int_0^\infty \frac{1}{\sqrt{m_e}} E \sigma_{ij}(E) e^{-E/kT_e} dE \quad (A1-19) \]

where \( m_e \) is the electron mass in grams.

\( T_e \) is the electron temperature in °K.

\( k \) is Boltzmann's constant.

Chen presents, in graphical form, the cross sections which allow calculation of (A1-19) for all transitions among the first five excited levels of \( N_2 \). Because we are concerned with moderate electron temperatures, the low energy regions of the cross sections are of particular interest. By using (A1-19) and detailed balancing arguments we may relate the cross sections for excitation and de-excitation in the following way

\[ \sigma_{ji} (E - \epsilon_{ij}) = \frac{E}{E - \epsilon_{ij}} \sigma_{ij}(E) \quad (A1-20) \]

where \( \epsilon_{ij} \) is the threshold for the \( j \rightarrow i \) transition. Thus, near threshold we should use de-excitation cross sections in (A1-19) because the low energy tails are more readily observed. The principal of detailed balance allows calculation of the excitation reaction rate from

\[ I_{ji} = I_{ij} e^{-(E_j - E_i)/kT_e} \quad (A1-21) \]

The cross-section graphs in Chen's paper (30) were digitized and numerical integration of (A1-19) was performed for electron temperatures between 500°K and 10000°K. The identification of the cross sections used are given in Table (1). The calculated reaction rates are plotted in Figures A1-1 through A1-15 as points.
Figure A1-1. Reaction rate constant calculated from $\sigma_{10}$
Figure A1.2. Reaction rate constant calculated from $\sigma_{20}$
Figure A1-3. Reaction rate constant calculated from $\sigma_{03}$.
Figure A1-4. Reaction rate constant calculated from $\sigma_{04}$.
Figure A1-5. Reaction rate constant calculated from $\sigma_{50}$
Figure A1-6. Reaction rate constant calculated from $\sigma_{12}$. 
Figure A1-7. Reaction rate constant calculated from $\sigma_{13}$
REACTION RATE CONSTANT FOR $\sigma_{14}$

Figure A1-8. Reaction rate constant calculated from $\sigma_{14}$
Figure A1.9. Reaction rate constant calculated from $\sigma_{51}$.
Figure A1-10. Reaction rate constant calculated from $\sigma_{23}$.
Figure A1-11. Reaction rate constant calculated from $\sigma_{24}$.
Figure A1-12. Reaction rate constant calculated from $\sigma_{52}$.
Figure A1-13. Reaction rate constant calculated from $\sigma_{34}$.
Figure A1-14. Reaction rate constant calculated from $\sigma_{53}$
Figure A1-15. Reaction rate constant calculated from $\sigma_{54}$
It was found that the reaction rates could be adequately reproduced by a four parameter function of the electron temperature of the form

$$I_{ij} = \exp \left( P_1 + \frac{P_2}{T_e} + \frac{P_3}{T_e^2} + \frac{P_4}{T_e^3} \right)$$  \hspace{1cm} (A1-22)

The four parameters for each cross section of Table (1) are given in Table (2).

Equation (A1-22) reproduces the integrated cross section results, over the electron temperature range, to better than 40% in all cases. This was considered acceptable considering the order of magnitude accuracy of the basic cross section calculations. The reaction rates from (A1-22) are also plotted as lines in Figures A1-1 through A1-15. Equations (A1-22) and (A1-21) were used to calculate the reaction rates used in further calculations.
APPENDIX II

SIMPLIFICATION OF THE CONTINUITY EQUATIONS

From section 2.4 we have for the continuity equation of the number of $N_2^*$ in level $i$

$$\frac{\partial n_i}{\partial t} + \frac{\partial}{\partial z} (n_i \nu) = \sum_{j=0}^{i-1} (A_{ij} n_j - A_{ji} n_i)$$

$$+ P_{1,0:0,1} \nu i \sum_{j=0}^{i+1} (j + 1) [n_{i-1} n_j + n_i n_j]$$

$$+ P_{1,0:0,1} \nu (i + 1) \sum_{j=1}^{i+1} j [n_{i+1} n_j - n_i n_j]$$

$$+ C_{1,0} \nu' n [0] [i n_{i-1} + (i + 1) e^{\theta/T} n_{i+1}]$$

$$+ (i e^{\theta/T} + i + 1) n_i$$  \hspace{1cm} (2-22)

These are a set of 6 coupled, non-linear, partial differential equations. The coefficients are functions of altitude through the altitudinal dependence of the model atmosphere and ionosphere parameters.

Each solution to equations (2-22) will be written as a sum of a Boltzmann distributed density, $n_i$, and a remainder term, $\epsilon_i$, to simplify the coupling between the equations. Thus,

$$n_i = n_i' + \epsilon_i$$  \hspace{1cm} (A2-1)

and we require that

$$\sum_{i=0}^{106} i n_i = \sum_{i=0}^{106} i n_i'$$  \hspace{1cm} (A2-2)
\[ \sum_{i=0}^{n} n_i = \sum_{i=0}^{n} n_i' = n \] (A2-3)

Equation (A2-2) and (A2-3), respectively, require the vibrational energy and density of the Maxwell-Boltzmann distributed density to be the energy and density of the solution for the set of equations (2-22). Thus, from equation (A2-1) we have using (A2-2) and (A2-3)

\[ \sum_{i=0}^{n} \epsilon_i = 0 \] (A2-4)

\[ \sum_{i=0}^{n} \epsilon_i' = 0 \] (A2-5)

Substituting (A2-1) into the flux term (A2-21) we obtain

\[ \vec{F}_i = \vec{F}_i' + \vec{G}_i' \] (A2-6)

where

\[ \vec{F}_i' = -D \left[ \nabla n_i' + \frac{n_i'}{H} \right] \] (A2-7)

\[ \vec{G}_i' = -D \left[ \nabla \epsilon_i' + \frac{\epsilon_i'}{H} \right] \] (A2-8)

Substituting (A2-1) into (2-22) and rearranging terms we have

\[ \frac{\partial n_i'}{\partial t} + \frac{\partial}{\partial z} (\vec{F}_i')_z + \frac{\partial \epsilon_i'}{\partial t} + \frac{\partial}{\partial z} (\vec{G}_i')_z = \sum_{j=0}^{A_{ij}} (n_j' + \epsilon_j) \]

\[ -A_{j1} (n_i' + \epsilon_i')) + P_{1,0;0,1} \nabla i \sum_{j=0}^{(j+1)} [n_{i-1}' n_{j+1}'] \]
\[ - n'_i n'_j + \varepsilon_{i-1} n'_{i+1} + \varepsilon_{i+1} n'_{i-1} - \varepsilon_i n'_j \]
\[ - \varepsilon_j n'_i + \varepsilon_{i-1} \varepsilon_{j+1} - \varepsilon_i \varepsilon_j \]
\[ + P_{1,0:0,1} \nu (i + 1) \sum_{j=1}^{j}[n'_{i+1} n'_{j-1} - n'_i n'_j] \]
\[ + \varepsilon_{i+1} n'_{j-1} + \varepsilon_{j-1} n'_{i+1} - \varepsilon_i n'_j - \varepsilon_j n' i \]
\[ + \varepsilon_{i+1} \varepsilon_{j-1} - \varepsilon_j \varepsilon_i] + C_{1,0} \nu' n [0] [i (n'_{i-1} + \varepsilon_{i-1})] \]
\[ + (i + 1) e^\theta/T (n'_{i+1} + \varepsilon_{i+1}) - (i e^\theta/T + i + 1) (n'_{i+1} + \varepsilon_{i+1}) \] (A2-9)

We have

\[ n'_{i-1} n'_{j+1} - n'_i n'_j = n'_{i+1} n'_{j-1} - n'_i n'_j \] (A2-10)

Using (A2-10) in (A2-9) and rearranging terms we have

\[ \frac{\partial n'_i}{\partial t} + \frac{\partial}{\partial x} (F'_i) + \frac{\partial \varepsilon_i}{\partial t} + \frac{\partial \Theta}{\partial z} = \sum_{j=0}^{j} (A_{i,j} (n'_j + \varepsilon_j)) \]
\[ + A_{jj} (n'_i + \varepsilon_i)] + P_{1,0:0,1} \nu \left[ i \varepsilon_{i-1} \sum_{j=0}^{j} (j + 1) n'_{j+1} \right] \]
\[ - (i + 1) \varepsilon_i \sum_{j=1}^{j} j n'_j + i n'_{i-1} \sum_{j=0}^{j} (j + 1) \varepsilon_{j+1} - (i + 1) n'_i \sum_{j=1}^{j} j \varepsilon_j \]
\[ - i \varepsilon_i \sum_{j=0}^{j} (j + 1) n'_j + (i + 1) \varepsilon_{i+1} \sum_{j=1}^{j} j n'_{j-1} - i n'_{i} \sum_{j=0}^{j} (j + 1) \varepsilon_j \]
+ (i + 1) n'_{i+1} \sum_{j=0}^{n} j \epsilon_{j-1} + i \epsilon_{i-1} \sum_{j=0}^{n} (j + 1) \epsilon_{j+1}

- (i + 1) \epsilon_{i} \sum_{j=1}^{n} j \epsilon_{j} - i \epsilon_{i} \sum_{j=0}^{n} (j + 1) \epsilon_{j} + (i + 1) \epsilon_{i+1} \sum_{j=1}^{n} j \epsilon_{j-1}

(A2-11)

+ C_{1,0} \nu' n [0 \left( n_{i-1}' + \epsilon_{i-1} \right) + (i + 1) \frac{\theta}{T} (n_{i+1}' + \epsilon_{i+1})]

- (i \frac{\theta}{T} + i + 1) \left( n_{i}' + \epsilon_{i} \right)

Using equations (A2-4) and (A2-5) in (A2-11) the 5th, 6th, 9th, 10th, 11th, 12th, 13th, and 14th terms on the right hand side are zero. Thus we have

\[
\frac{\partial n_{i}'}{\partial t} + \frac{\partial}{\partial z} \left( \tilde{F}_{i}' \right) + \frac{\partial}{\partial z} \left( \tilde{\beta}_{i} \right) = \sum_{j=0}^{n} \left( A_{ij} \left( n_{j}' + \epsilon_{j} \right) \right)

- A_{ji} \left( n_{i}' + \epsilon_{i} \right) + P_{1,0;0,1} \nu \left[ \left\{ i \epsilon_{i-1} - (i + 1) \epsilon_{i} \right\} \sum_{j=1}^{n} j n_{j}' \right]

+ \left\{ (i + 1) \epsilon_{i+1} - i \epsilon_{i} \right\} \sum_{j=1}^{n} j n_{j-1}' \right] + C_{1,0} \nu' n [0 \left( n_{i-1}' + \epsilon_{i-1} \right)]

+ (i + 1) \frac{\theta}{T} \left( n_{i+1}' + \epsilon_{i+1} \right) - (i \frac{\theta}{T} + i + 1) \left( n_{i}' + \epsilon_{i} \right)

(A2-12)

A.2.1 The equation for the Boltzmann part of the solution.

Multiply (A2-12) by i and sum over i to get
\[
\frac{\partial}{\partial t} \sum_{i=0}^{n_i'} \nabla_i \left( \sum_{i=0}^{n_i} F'_i \right) = \sum_{i=0}^{n_i} \sum_{j=0}^{n_j} \left\{ A_{ij} (n_j' + \epsilon_j) \right. \\
\left. - A_{ji} (n_i' + \epsilon_i) \right\} + P_{1,0:0,1} \nu \left[ \sum_{j=1}^{n_j} j n_j' \left\{ \sum_{i=0}^{n_i} [i^2 \epsilon_{i-1} - (i + 1) \epsilon_i] \right\} \right. \\
\left. + \sum_{j=1}^{n_j} j n_{j-1}' \left\{ \sum_{i=0}^{n_i} [i (i + 1) \epsilon_{i+1} - i^2 \epsilon_i] \right\} \right\] \\
(A2-13) \\
+ C_{1,0} \nu' n \left[ \sum_{i=0}^{n_i} \{i^2 n_{i-1}' + i (i + 1) e^\theta/T n_{i+1}' \right. \\
\left. - i (i e^\theta/T + i + 1) n_i' \} + \sum_{i=0}^{n_i} \{i^2 \epsilon_{i-1} - i (i + 1) \epsilon_i \right\} \\
+ \epsilon^\theta/T \sum_{i=0}^{n_i} \{i (i + 1) \epsilon_{i+1} - i^2 \epsilon_i \left. \right\} \right]
\]

where we have used (A2-4) and

\[
\sum_{i=0}^{n_i} i \bar{\nabla}_i = - \sum_{i=0}^{n_i} i D \left[ \nabla \epsilon_i + \frac{\epsilon_i}{k} \right] \\
= - D \left[ \nabla \sum_{i=0}^{n_i} i \epsilon_i + \sum_{i=0}^{n_i} i \frac{\epsilon_i}{k} \right] \\
= 0 \\
(A2-14)
\]

Consider

\[
\sum_{i=0}^{n_i} \{i^2 \epsilon_{i-1} - i (i + 1) \epsilon_i \} = \sum_{i=1}^{n_i} i^2 \epsilon_{i-1} - \sum_{i=0}^{n_i} i^2 \epsilon_i - \sum_{i=0}^{n_i} i \epsilon_i \\
= \sum_{i=0}^{n_i} (i + 1)^2 \epsilon_i - \sum_{i=0}^{n_i} i^2 \epsilon_i
\]
\[111\]

\[= \sum_{i=0}^{\infty} (2i + 1) \epsilon_i \quad \text{(A2-15)}\]

\[= 0\]

Also consider

\[
\sum_{i=0} \left[ i(i+1) \epsilon_{i+1} - i^2 \epsilon_i \right] = \sum_{i=0} i(i-1) \epsilon_i - \sum_{i=0} i^2 \epsilon_i
\]

\[= -\sum_{i=0} i \epsilon_i\]

\[= 0 \quad \text{(A2-16)}\]

Using (A2-15) and (A2-16) in (A2-13) we have

\[
\frac{\partial}{\partial t} \sum_{i=0} i n_i' + \frac{\partial}{\partial z} \left( \sum_{i=0} i \tilde{F}_i' \right) = \sum_{i=0} \sum_{j=0} i (A_{ij} (n_j' + \epsilon_j) - A_{ji} (n_i' + \epsilon_i)) + C_{1,0} \nu' [0] \sum_{i=0} i^2 n_{i-1}'
\]

\[+ i (i+1) e^{\beta/T} n_{i+1}' - i (i e^{\beta/T} + i + 1) n_i' \quad \text{(A2-17)}\]

Consider

\[
\sum_{i=0} \left\{ i^2 n'_{i-1} + i (i+1) e^{\beta/T} n_{i+1}' - i (i e^{\beta/T} + i + 1) n_i' \right\}
\]

\[= \sum_{i=0} \left\{ (i+1)^2 n_i' - i^2 n_i' - i n_i' + e^{\beta/T} \{ i (i - 1) n_i' - i^2 n_i' \} \right\}\]
\[
\begin{align*}
\sum_{i=0}^{\infty} \left\{ (i + 1) - i \frac{e^{\theta/T}}{T} \right\} n_i' &= (A2-18) \\

\text{Therefore equation (A2-17) becomes}
\end{align*}
\]

\[
\begin{align*}
\frac{\partial}{\partial t} \sum_{i=0}^{\infty} i n_i' + \frac{\partial}{\partial z} \left( \sum_{i=0}^{\infty} \frac{z}{i} \right) &= \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} i \{ A_{ij} (n_i' + \epsilon_j) \\
&- A_{ji} (n_j' + \epsilon_i) \} + C_{1,0} \nu' n [0] \sum_{i=0}^{\infty} (i + 1) n_i' \\
&- \frac{e^{\theta/T}}{T} \sum_{i=0}^{\infty} i n_i' \\
&= (A2-19)
\end{align*}
\]

Let \( Z_p \) be the partition function for the Boltzmann distributed part of the solution.

Then,

\[
Z_p = \frac{1}{1 - e^{-a}}
\]

where

\[
a = \frac{\theta}{T_v}
\]

and \( T_v \) is the vibrational temperature. Therefore

\[
\sum_{i=0}^{\infty} i n_i' = \sum_{i=0}^{\infty} i \frac{n}{Z_p} e^{-a} \\
= \frac{n}{Z_p} \frac{e^{-a}}{(1 - e^{-a})^2} \\
= n (Z_p - 1)
\]

(A2-23)
Also

\[ \sum_{i=0} \vec{F}_i = -D \left[ \nabla \sum_{i=0} n_i + \sum_{i=0} \frac{n_i}{H} \right] \]
\[ = -D \left[ \nabla n (Z_p - 1) + \frac{n (Z_p - 1)}{H} \right] \]  
(A2-24)

Consider

\[ \sum_{i=0} \sum_{j=0} \left\{ A_{ij} (n_j + \epsilon_j) - A_{ji} (n_i + \epsilon_i) \right\} = (n_0' + \epsilon_0) \left\{ \sum_{i=0} A_{i0} (1 - \delta_{i0}) \right\} \]
\[ + (n_1' + \epsilon_1) \left\{ \sum_{i=0} A_{i1} (1 - \delta_{i1}) - \sum_{j=0} A_{j1} (1 - \delta_{1j}) \right\} \]
\[ + (n_2' + \epsilon_2) \left\{ \sum_{i=0} A_{i2} (1 - \delta_{i2}) - \sum_{j=0} 2A_{j2} (1 - \delta_{j2}) \right\} \]
\[ + \ldots \]
\[ + (n_k' + \epsilon_k) \left\{ \sum_{i=0} A_{ik} (1 - \delta_{ik}) - \sum_{j=0} A_{jk} (1 - \delta_{jk}) \right\} \]
\[ + \ldots \]
\[ = (n_0' + \epsilon_0) \left\{ \sum_{i=0} (1 - \delta_{i0}) A_{i0} + (n_1' + \epsilon_1) \sum_{i=0} (i - 1) A_{i1} \right\} \]
\[ + (n_2' + \epsilon_2) \left\{ \sum_{i=0} (i - 2) A_{i2} \right\} + \ldots \]
\[ + (n_k' + \epsilon_k) \left\{ \sum_{i=0} (i - k) A_{ik} \right\} + \ldots \]
\[ = \sum_{i=0} \sum_{j=0} (n_j' + \epsilon_j) (i - j) A_{ij} \]  
(A2-25)
Using (A2-23), (A2-24) and (A2-25) in equation (A2-19) we have

\[
\frac{\partial}{\partial t} n (Z_p - 1) + \frac{\partial}{\partial z} \left\{ - D \left[ \frac{\partial}{\partial z} n (Z_p - 1) + \frac{n (Z_p - 1)}{H} \right] \right\} = \sum_{i=0}^{n} \sum_{j=0}^{n} (n_j' + \epsilon_j) (i - j) A_{ij}
\]

\[+ C_{1,0} \nu' n [0] [n (Z_p - 1) + n - e^{\theta/T} n (Z_p - 1)] \quad (A2-26)\]

Let

\[\psi = (Z_p - 1) \quad (A2-27)\]

and use

\[\frac{\partial n}{\partial t} = 0\]

and

\[(Z_p - 1) \frac{\partial n}{\partial z} = - \frac{n (Z_p - 1)}{H}\]

in equation (A2-26) to obtain

\[n \frac{\partial \psi}{\partial t} + \frac{\partial}{\partial z} \left( - D n \frac{\partial \psi}{\partial z} \right) = \sum_{i=0}^{n} \sum_{j=0}^{n} (n_j' + \epsilon_j) (i - j) A_{ij}\]

\[+ C_{1,0} \nu' n [0] n [\psi + 1 - e^{\theta/T} \psi] \quad (A2-28)\]

Using

\[n_j' = \frac{n}{Z_p} (e^{-\alpha})^j\]

\[= \frac{n}{\psi + 1} \left( \frac{\psi}{\psi + 1} \right)^j \quad (A2-29)\]
and dividing equation (A2-28) by \( n \) we have

\[
\frac{\partial \psi}{\partial t} - \frac{1}{n} \left( \frac{\partial D n}{\partial z} \right) \frac{\partial \psi}{\partial z} - D \frac{\partial \psi^2}{\partial z^2} = \sum_{i=0}^{n} \sum_{j=0}^{n} \left[ \frac{1}{\psi + 1} \left( \frac{\psi}{\psi + 1} \right)^j + \frac{\epsilon_j}{n} \right]
\]

\[ (i - j) A_{ij} + C_{1,0} \nu' n [0] \cdot [\psi + 1 - e^{\theta/T} \psi]. \]  

(A2-30)

The boundary conditions become for: set 1;

initial condition: \( \psi(z, 0) = 0 \)

lower boundary: \( \psi(120, t) = 0 \)

upper boundary: \( \frac{\partial n}{\partial z} - \frac{n}{H} \Rightarrow \frac{\partial n}{\partial z} + \frac{\partial \epsilon_i}{\partial z} = - \frac{n}{H} - \frac{\epsilon_i}{H} \)

Using (A2-23)

\[
\frac{\partial}{\partial z} \sum_{i=p}^{n} i n_i' = - \sum_{i=0}^{n} i \frac{n_i'}{H}
\]

Using (A2-23) and (A2-27) we have

\[
\frac{\partial}{\partial z} n \psi \bigg|_{z=\infty} = - \frac{n \psi}{H} \bigg|_{z=\infty} \]  

(A2-31)

Thus,

\[
\frac{\partial \psi}{\partial z} \bigg|_{z=0} = 0
\]

set 2;

initial condition: \( \psi(z, 0) = \frac{e^{-\theta/355}}{1 - e^{-\theta/355}} \)

\[ = 7.329241 \times 10^{-5} \]
lower boundary: \[ \psi (0, t) = 7.329241 \times 10^{-5} \]

upper boundary: \[ \frac{\partial \psi}{\partial z} = 0 \] (A2-32)

It is worthy of note that the only coupling between equation (A2-30) and the other equations is through the \( \epsilon_j / n \) term of the source of \( N^* \) due to electron collisions. This fact, and the expectation that \( \epsilon_j / n \) is small with respect to 1 for all \( j \) of interest, will be exploited in the solution of (A2-30).

A2.2 The equations for the deviation parts of the solution.

Returning to equation (A2-12) for the \( \epsilon_i \)'s and treating the \( n_j \)'s as known quantities we have

\[
\frac{\partial}{\partial t} \epsilon_i + \frac{\partial}{\partial z} (\bar{\psi}_i) = \sum_{j=0} \{ A_{ij} (n_j' + \epsilon_j) - A_{ji} (n_i' + \epsilon_i) \} - \frac{\partial n_i'}{\partial t} \\
- \frac{\partial}{\partial z} \psi_i' + \sum_{i=0} P_{1,0:0,1} \nu \left[ \{i \epsilon_{i-1} - (i + 1) \epsilon_i\} \sum_j j n_j \\
+ \{ (i + 1) \epsilon_{i+1} - i \epsilon_i \} \sum_{j=-1} \bar{n}_{j-1} \} + C_{1,0} \nu' n [0] [i \epsilon_{i-1} \\
+ \epsilon_{i-1} + (i + 1) \epsilon_{i+1} + (i + 1) \epsilon_i / T (n_{i+1}' + \epsilon_{i+1}) - (i \epsilon_i) / T + i + 1) \\
\cdot \bar{n}_{i+1} \}
\]

Using equations (A2-23) and (A2-27) we have

\[
\frac{\partial}{\partial t} \epsilon_i + \frac{\partial}{\partial z} (\bar{\psi}_i) = \sum_{j=0} \{ A_{ij} (n_j' + \epsilon_j) - A_{ji} (n_i' + \epsilon_i) \} - \frac{\partial n_i'}{\partial t} \\
- \frac{\partial}{\partial z} \psi_i' + \sum_{i=0} P_{1,0:0,1} \nu \left[ \{i \epsilon_{i-1} - (i + 1) \epsilon_i\} \bar{n} \psi \right.
\]
+ \{(i + 1) \epsilon_{i+1} - i \epsilon_i\} n (\psi + 1) \]

\[ + c_{1,0} \nu' n [0] \cdot i \left( n_{i-1} + \epsilon_{i-1} \right) + (i + 1) e^{\theta/T} \left( n_{i+1} + \epsilon_{i+1} \right) \]

\[ - (i e^{\theta/T} + i + 1) \left( n_i' + \epsilon_i' \right) \]. \tag{A2-34} \]

Rearranging terms in (A2-34) and dividing by \( n_i' \), we have

\[ \frac{1}{n_i'} \frac{\partial}{\partial t} \epsilon_i + \frac{1}{n_i'} \frac{\partial}{\partial n_i'} \left( \frac{\nabla_i'}{\nabla_i} \right) \sum_{j=0}^1 \left\{ A_{ij} \left( \frac{n_j''}{n_i'} + \frac{\epsilon_i n_j'}{n_i'} \right) - A_{ij+1} \left( 1 + \frac{\epsilon_i}{n_i'} \right) \right\} \]

\[ - \frac{1}{n_i'} \frac{\partial}{\partial t} n_i' - \frac{1}{n_i'} \frac{\partial}{\partial \nabla_i} \left( \frac{\nabla_i'}{\nabla_i} \right) \left[ P_{1,0:0,1} \nu n \left( (2 i + 1) \psi + i \right) + i \right] + C_{1,0} \nu' n [0] \cdot (i e^{\theta/T} + i + 1) \]

\[ + \frac{\epsilon_{i-1}}{n_{i-1}'} \frac{n_{i-1}'}{n_i'} \left[ P_{1,0:0,1} \nu i n \psi + C_{1,0} \nu' n [0] \cdot i \right] \]

\[ + \frac{\epsilon_{i+1}}{n_{i+1}'} \frac{n_{i+1}'}{n_i'} \left[ P_{1,0:0,1} \nu n \left( i + 1 \right) \left( \psi + 1 \right) + C_{1,0} \nu' n [0] \cdot e^{\theta/T} \left( i + 1 \right) \right] \]

\[ + C_{1,0} \nu' n [0] \left[ i \frac{n_{i-1}'}{n_i'} + (i + 1) e^{\theta/T} \frac{n_{i+1}'}{n_i'} - (i e^{\theta/T} + i + 1) \right] \] \tag{A2-35} \]

Consider

\[ \frac{\partial}{\partial t} \frac{\epsilon_i}{n_i'} = \frac{1}{n_i'} \frac{\partial}{\partial t} \epsilon_i - \frac{\epsilon_i}{(n_i')^2} \frac{\partial}{\partial t} n_i' \]

thus

\[ \frac{1}{n_i'} \frac{\partial}{\partial t} \epsilon_i = \frac{\partial}{\partial t} \frac{\epsilon_i}{n_i'} + \frac{1}{n_i'} \frac{\epsilon_i}{n_i'} \frac{\partial}{\partial t} n_i' \] \tag{A2-36}
Also

\[ \nabla \frac{\varepsilon_i}{n_i'} = \frac{1}{n_i'} \nabla \varepsilon_i - \frac{\varepsilon_i}{(n_i')^2} \nabla n_i' \]

Therefore

\[ \nabla \varepsilon_i = n_i' \nabla \frac{\varepsilon_i}{n_i'} + \frac{\varepsilon_i}{n_i'} \nabla n_i' \]

Therefore

\[ \frac{1}{n_i'} \frac{\partial}{\partial z} (\vec{y}_i)_z = \frac{1}{n_i'} \frac{\partial}{\partial z} \left[ -D \left\{ \frac{\partial \varepsilon_i}{\partial z} + \frac{\varepsilon_i}{H} \right\} \right] \]

\[ = \frac{1}{n_i'} \frac{\partial}{\partial z} \left[ -D \left\{ n_i' \frac{\partial \varepsilon_i}{\partial z} n_i' + \frac{\varepsilon_i}{n_i'} \frac{\partial n_i'}{\partial z} + \frac{\varepsilon_i}{n_i'} \right\} \right] \]

\[ = \frac{1}{n_i'} \frac{\partial}{\partial z} \left[ -Dn_i' \frac{\partial \varepsilon_i}{\partial z} n_i' - D \frac{\varepsilon_i}{n_i'} \left\{ \frac{\partial n_i'}{\partial z} + \frac{n_i'}{H} \right\} \right] \quad (A2-38) \]

Let

\[ \varphi_i = \frac{\varepsilon_i}{n_i'} \quad (A2-39) \]

then (A2-36) and (A2-38) become, respectively,

\[ \frac{1}{n_i'} \frac{\partial \varepsilon_i}{\partial t} = \frac{\partial}{\partial t} \varphi_i + \frac{1}{n_i'} \varphi_i \frac{\partial}{\partial t} n_i' \quad (A2-40) \]

and

\[ \frac{1}{n_i'} \frac{\partial}{\partial z} (\vec{y}_i)_z = \frac{1}{n_i'} \frac{\partial}{\partial z} \left[ -Dn_i' \frac{\partial \varphi_i}{\partial z} n_i' - D\varphi_i \left\{ \frac{\partial n_i'}{\partial z} + \frac{n_i'}{H} \right\} \right] \quad (A2-41) \]

Using (A2-39), (A2-40), (A2-41) in (A2-35) and rearranging terms we have

\[ \frac{\partial}{\partial t} \varphi_i - D \frac{\partial^2}{\partial z^2} \varphi_i - \left[ \frac{1}{n_i'} \frac{\partial}{\partial z} Dn_i' + \frac{1}{n_i'} D \left\{ \frac{\partial n_i'}{\partial z} + \frac{n_i'}{H} \right\} \right] \frac{\partial \varphi_i}{\partial z} \]

\[ + \left[ \frac{1}{n_i'} \frac{\partial}{\partial t} n_i' - \frac{1}{n_i'} \frac{\partial}{\partial z} \left\{ D \left( \frac{\partial n_i'}{\partial z} + \frac{n_i'}{H} \right) \right\} \right] + \sum_{j=0} A_{ji} (1 - \delta_{ij}) \]

\[ + P_{1,0} \nu \nu (2i + 1) \psi + i) + C_{1,0} \nu \nu' n [0] (i e^{\alpha T} + i + 1) \] \[ \varphi_i \]
\[
\begin{align*}
\sum_{j=0} \left\{ A_{ij} (1 + \varphi_j) e^{-j(j-1)} \psi / T - A_{ij} \right\} (1 - \delta_{ij}) - \frac{1}{n_i'} \frac{\partial n_i'}{\partial t} \\
- \frac{1}{n_i'} \frac{\partial}{\partial z} \left\{ - D \left( \frac{\partial n_i'}{\partial z} + \frac{n_i'}{H} \right) \right\} + \varphi_i e^{\psi / T} [P_{i,0:0,1}, \nu n_i \psi ] \\
+ C_{i,0} \nu' [0, i] + \varphi_i e^{-\psi / T} [P_{i,0:0,1}, \nu n(i + 1) (\psi + 1)] \\
+ C_{i,0} \nu' [0, i] e^{\psi / T} (i + 1)] + C_{i,0} \nu' [0, i] + (i + 1) e^{\psi / T - \psi / T} - (i e^{\psi / T + i + 1})
\end{align*}
\]

(A2-42)

Consider

\[
\frac{1}{n_j'} \frac{\partial n_j'}{\partial y} \quad \text{where} \quad n_j' = n \frac{\psi^j}{(\psi + 1)^{j+1}}
\]

\[
\frac{1}{n_j'} \frac{\partial n_j'}{\partial y} = \frac{1}{n} \frac{\partial n}{\partial y} + \left\{ \frac{j - j + 1}{\psi - \psi + 1} \right\} \frac{\partial \psi}{\partial y}
\]

(A2-43)

Thus, if \( y = t \)

\[
\frac{1}{n_j'} \frac{\partial n_j'}{\partial t} = \left( \frac{j - j + 1}{\psi - \psi + 1} \right) \frac{\partial \psi}{\partial t}
\]

(A2-44)

and if \( y = z \)

\[
\frac{1}{n_j'} \frac{\partial n_j'}{\partial z} = - \frac{1}{H} + \left( \frac{j - j + 1}{\psi - \psi + 1} \right) \frac{\partial \psi}{\partial z}
\]

(A2-45)

Using (A2-44) and (A2-45) in (A2-42) and collecting terms we have
\[
\frac{\partial}{\partial t} \varphi_i - D \frac{\partial^2}{\partial z^2} \varphi_i - \left[ \frac{\partial D}{\partial z} + D \left( -\frac{1}{H} + 2 \left\{ \frac{i}{\psi} - \frac{i+1}{\psi+1} \right\} \frac{\partial \psi}{\partial z} \right) \right] \frac{\partial \varphi_i}{\partial z} \\
+ \left\{ \frac{i}{\psi} - \frac{i+1}{\psi+1} \right\} \frac{\partial \psi}{\partial t} - \frac{\partial \psi}{\partial z} \left\{ \frac{i}{\psi} - \frac{i+1}{\psi+1} \right\} \left\{ \frac{\partial D}{\partial z} + D \left( -\frac{1}{H} \right) \right\} \\
+ \left\{ \frac{i}{\psi} - \frac{i+1}{\psi+1} \right\} \frac{\partial^2 \psi}{\partial z^2} - D \left\{ \frac{i}{\psi} - \frac{i+1}{\psi+1} \right\} \frac{\partial^2 \psi}{\partial z^2} - D \left( \frac{\partial \psi}{\partial z} \right)^2 \left\{ \frac{i}{\psi^2} \right\} \\
+ \frac{(i+1)}{(\psi+1)^2} \sum_{j=0}^{\infty} A_{ji} (1 - \delta_{ij}) + P_{1,0:0,1} \varphi_n \left\{ (2i + 1) \psi + i \right\} \\
+ C_{1,0} \nu' n[0] \left( i e^{\theta/T} + i + 1 \right) \varphi_i = \sum_{j=0}^{\infty} \left\{ A_{ij} (1 + \varphi_j) e^{-\left( j-i \right) \theta/Tv} \right\} (1 - \delta_{ij}) \\
- \left[ \left( \frac{i}{\psi} - \frac{i+1}{\psi+1} \right) \frac{\partial \psi}{\partial t} - \frac{\partial \psi}{\partial z} \left( \frac{i}{\psi} - \frac{i+1}{\psi+1} \right) \left\{ \frac{\partial D}{\partial z} + D \left( -\frac{1}{H} \right) \right\} \\
+ \left( \frac{i}{\psi} - \frac{i+1}{\psi+1} \right) \frac{\partial^2 \psi}{\partial z^2} \sum_{j=0}^{\infty} A_{ji} (1 - \delta_{ij}) - D \left( \frac{i}{\psi} - \frac{i+1}{\psi+1} \right) \frac{\partial^2 \psi}{\partial z^2} \\
- D \left( \frac{\partial \psi}{\partial z} \right)^2 \left\{ \frac{i}{\psi^2} + \frac{i+1}{(\psi+1)^2} \right\} + P_{1,0:0,1} \varphi_n \left\{ (2i + 1) \psi + i \right\} \\
+ C_{1,0} \nu' n[0] \left( i e^{\theta/T} + i + 1 \right) \varphi_i = \sum_{j=0}^{\infty} \left\{ A_{ij} (1 + \varphi_j) e^{-\left( j-i \right) \theta/Tv} \right\} + P_{1,0:0,1} \varphi_n \left\{ (2i + 1) \psi + i \right\} \\
+ C_{1,0} \nu' n[0] \left[ i e^{\theta/Tv} + (i + 1) e^{\theta/T-\theta/Tv} \right] + \varphi_{i-1} e^{\theta/Tv} \left[ P_{1,0:0,1} \nu n_i \psi \right] \\
+ C_{1,0} \nu' n[0] i + \varphi_{i+1} e^{-\theta/Tv} \left[ P_{1,0:0,1} \nu n_{i+1}(\psi+1) \right] \\
+ C_{1,0} \nu' n[0] e^{\theta/T} (i + 1) \right\} \\
\quad \text{(A2-46)}
The boundary conditions for the $\epsilon_i$'s are, by assumption, identical for set 1 and set 2 boundary conditions for $\psi$. For

initial condition $\phi_i(z, 0) = 0$ for all $i$

lower boundary $\phi_i(120, t) = 0$ for all $i$

upper boundary $\frac{\partial n_i}{\partial z} = -\frac{n_i}{H}$

thus,

$$\frac{\partial n_i'}{\partial z} + \frac{\partial \epsilon_i}{\partial z} = -\frac{n_i'}{H} - \frac{\epsilon_i}{H}$$

using (A2-45)

$$n_i' \left[ -\frac{1}{H} + \left(\frac{i}{\psi} - \frac{i + 1}{\psi + 1}\right) \frac{\partial \psi}{\partial z} \right] + \frac{\partial \epsilon_i}{\partial z} = -\frac{n_i'}{H} - \frac{\epsilon_i}{H}$$

thus

$$n_i' \left\{ \frac{i}{\psi} - \frac{i + 1}{\psi + 1} \right\} \frac{\partial \psi}{\partial z} + \frac{\partial \epsilon_i}{\partial z} = -\frac{\epsilon_i}{H}$$

using equation (A2-32) we obtain

$$\left. \frac{\partial \epsilon_i}{\partial z} \right|_{z=\infty} = -\frac{\epsilon_i}{H} \bigg|_{z=\infty}$$

now using (A2-37) and (A2-39) we have

$$n_i' \frac{\partial}{\partial z} \phi_i + \phi_i \frac{\partial n_i}{\partial z} = -\phi_i \frac{n_i'}{H}$$

thus, using (A2-45)

$$n_i' \frac{\partial}{\partial z} \phi_i + \phi_i n_i' \left\{ -\frac{1}{H} + \left(\frac{i}{\psi} - \frac{i + 1}{\psi + 1}\right) \frac{\partial \psi}{\partial z} \right\} = -\phi_i \frac{n_i'}{H}$$
again using (A2-32) we have:

$$\left[ n_i' \frac{\partial \varphi_i}{\partial z} \right]_{z=\infty} = 0$$

or

$$\left. \frac{\partial \varphi_i}{\partial z} \right|_{z=\phi} = 0 \quad \text{for all } i \quad (A2-47)$$

From equation (A2-46) it is seen that all solutions are coupled through the electronic source term and that only those levels adjacent to the level of interest are coupled through vibration-vibrational or vibrational-translational energy exchange terms. If \( \psi \) is assumed known, then equation (A2-46) represents a set of 6, coupled, linear, partial differential equations for the \( \epsilon_i \)'s.
To numerically solve equations (A2-30) and (A2-46) we will use the finite difference approximation of Crank and Nicholson (see reference (36)). This particular choice was made because, in a linear problem, the errors are of order two in both the time and space step, and the solutions are expected to be unconditionally stable.

A3.1 Finite difference form, the \( \psi \) equation.

Equation (A2-30) becomes in six point finite difference form with

\[
\psi_{\ell}^m = \psi((\ell - 1) \Delta z, (m - 1) \Delta t) \quad \ell = 1, 2, \cdots, L
\]

\[
m = 1, 2, \cdots, M
\tag{A3-1}
\]

where \( \Delta z \) is the altitudinal space step size and \( \Delta t \) is the time step size

\[
\frac{\psi_{\ell}^{m+1} - \psi_{\ell}^m}{\Delta t} = \frac{1}{n \ell} \left( \frac{\partial Dn}{\partial z} \right)_\ell \frac{1}{2\Delta z} \left\{ \psi_{\ell+1}^m - \psi_{\ell-1}^m \right\} - \frac{D \ell}{2(\Delta z)^2} \left\{ \psi_{\ell+1}^{m+1} - 2\psi_{\ell}^{m+1} + \psi_{\ell-1}^{m+1} + \psi_{\ell+1}^m - 2\psi_{\ell}^m + \psi_{\ell-1}^m \right\}
\]

\[
= \sum_{j=0}^{\ell} \sum_{i=0}^{\ell} \left[ \frac{1}{\psi_{\ell}^m + 1} \left( \frac{\psi_{\ell}^m}{\psi_{\ell}^m + 1} \right)^j + \frac{\epsilon_j}{n} \right] (i - j) A_{i,j}
\tag{A3-2}
\]

and the subscript \( \ell \) and superscript \( m \) mean that the quantities are evaluated at the altitude \( 120 + (\ell - 1) \Delta z \) and time \( \sum_{i=1}^{m} (m-1) \Delta t \), respectively. The term \( \epsilon_j / n \) has been retained in the source term in (A3-2) for completeness. Solving for the \( m+1 \) superscripted terms in (A3-2) we have
\[- \frac{D \Delta t}{2(\Delta z)^2} \psi_{\ell+1}^{m+1} + \left\{ 1 + \frac{D \Delta t}{(\Delta z)^2} \right\} \psi_{\ell}^{m+1} - \frac{D \Delta t}{2(\Delta z)^2} \psi_{\ell-1}^{m+1} \]

\[= \left\{ \frac{D \Delta t}{2(\Delta z)^2} + \frac{1}{n \ell} \left( \frac{\partial Dn}{\partial z} \right) \frac{\Delta t}{2\Delta z} \right\} \psi_{\ell+1}^{m} \]

\[+ \left\{ 1 - \frac{D \Delta t}{(\Delta z)^2} \right\} \psi_{\ell}^{m} + \left\{ \frac{D \Delta t}{2(\Delta z)^2} - \frac{1}{n \ell} \left( \frac{\partial Dn}{\partial z} \right) \frac{\Delta t}{2\Delta z} \right\} \psi_{\ell-1}^{m} \]

\[+ \Delta t \sum_{j=0} \sum_{i=0} \left[ \frac{1}{\psi_{\ell}^{m} + 1} \left( \frac{\psi_{\ell}^{m}}{\psi_{\ell}^{m} + 1} \right)^{j} + \frac{\ell c_{i}}{n} \right] (i - j) A_{i j} \quad (A3-3) \]

Let

\[A_{\ell} = \frac{D \Delta t}{2(\Delta z)^2} \quad (A3-4)\]

\[B_{\ell} = 1 + \frac{D \Delta t}{(\Delta z)^2} \]

\[= 1 + 2 A_{\ell} \quad (A3-5)\]

\[D_{\ell} = \left\{ A_{\ell} + \frac{1}{n \ell} \left( \frac{\partial Dn}{\partial z} \right) _{\ell} \frac{\Delta t}{\Delta z} \right\} \psi_{\ell+1}^{m} + \{ 1 - 2 A_{\ell} \} \psi_{\ell}^{m} \]

\[+ \left\{ A_{\ell} - \frac{1}{n \ell} \left( \frac{\partial Dn}{\partial z} \right) _{\ell} \frac{\Delta t}{2\Delta z} \right\} \psi_{\ell-1}^{m} \]

\[+ \Delta t \sum_{j=0} \sum_{i=0} \left[ \frac{1}{\psi_{\ell}^{m} + 1} \left( \frac{\psi_{\ell}^{m}}{\psi_{\ell}^{m} + 1} \right)^{j} + \frac{\ell c_{i}}{n} \right] (i - j) A_{i j} \quad (A3-6) \]

Thus (A3-3) becomes

\[- A_{\ell} \psi_{\ell+1}^{m+1} + B_{\ell} \psi_{\ell}^{m+1} - A_{\ell} \psi_{\ell-1}^{m+1} = D_{\ell}^{m} \quad (A3-7)\]
The boundary conditions become

<table>
<thead>
<tr>
<th>Set 1</th>
<th>Set 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m = 1$</td>
<td>$\psi^1_L = 0$</td>
</tr>
<tr>
<td>$\ell = 1$</td>
<td>$\psi^1_1 = 7.329241 \times 10^{-5}$</td>
</tr>
</tbody>
</table>

(A3-8) $\ell = L$ $\psi^m_L - \psi^m_{L-1} = 0$ $\psi^m_L - \psi^m_{L-1} = 0$ (A3-9)

A3.2 Finite difference form, the $\varphi_i$ equations.

Let

$$\lambda^m_{\alpha i} = \left[ \frac{\partial D}{\partial z} + D \left( -\frac{1}{H} + 2 \left\{ \frac{i}{\psi} - \frac{i + 1}{\psi + 1} \right\} \frac{\partial \psi}{\partial z} \right) \right]_{\ell, m} \quad (A3-10)$$

$$\lambda^m_{\beta i} = \left[ \left( \frac{i}{\psi} - \frac{i + 1}{\psi + 1} \right) \frac{\partial \psi}{\partial z} - \frac{\partial \psi}{\partial z} \left\{ \frac{i}{\psi} - \frac{i + 1}{\psi + 1} \right\} \right] \frac{\partial D}{\partial z}$$

$$+ D \left( -\frac{1}{H} + \left\{ \frac{i}{\psi} - \frac{i + 1}{\psi + 1} \right\} \frac{\partial \psi}{\partial z} \right) - D \left\{ \frac{i}{\psi} - \frac{i + 1}{\psi + 1} \right\} \frac{\partial^2 \psi}{\partial z^2}$$

$$- D \left( \frac{\partial \psi}{\partial z} \right)^2 \left\{ -\frac{i}{\psi^2} + \frac{(i + 1)}{(\psi + 1)^2} \right\} + \sum_{j=0}^{\ell, m} A_{ij} \left( 1 - \delta_{ij} \right)$$

$$+ P_{i, 0; 0, 1} \nu n (2i + 1) \psi + i + C_{1, 0} \nu' n[0] (i e^{\theta/T} + i + 1) \right] \quad (A3-11)$$

$$\lambda^m_{\gamma i} = \left[ \sum_{j=0} \left\{ A_{ij} \left( 1 + \varphi_j \right) e^{-(i-j) \theta/T} \nu \left( 1 - \delta_{ij} \right) - \frac{\partial \psi}{\partial z} \right\} \right]_{\ell, m}$$

$$+ P_{i, 0; 0, 1} \nu n (2i + 1) \psi + i + C_{1, 0} \nu' n[0] \left\{ i e^{\theta/T} \right\}$$

$$+ (i + 1) e^{\theta/T} \nu n[0] \left\{ i e^{\theta/T} \right\} + \varphi_{i-1} e^{\theta/T} \nu n[0] \nu \psi$$

$$+ C_{1, 0} \nu' n[0] i + C_{1, 0} \nu' n[0] e^{-\theta/T} \nu n[1] (i + 1) \psi + 1$$

$$+ C_{1, 0} \nu' n[0] e^{\theta/T} (i + 1) \right] \quad (A3-12)$$
Using (A3-10) through (A3-12) and expressing (A2-46) in finite difference form we have after some rearrangement of terms

\[ -\frac{D_\ell \Delta t}{2(\Delta z)^2} \lambda_{i+1}^{m+1} + \left[ \frac{D_\ell \Delta t}{(\Delta z)^2} + 1 \right] \lambda_{i}^{m+1} \quad + \frac{D_\ell \Delta t}{2(\Delta z)^2} \lambda_{i-1}^{m+1} \]

\[ = \left[ \frac{D_\ell \Delta t}{2(\Delta z)^2} + \lambda_{i}^{m} \frac{\Delta t}{2\Delta z} \right] \lambda_{i}^{m} + \left[ 1 - \frac{D_\ell \Delta t}{(\Delta z)^2} \right] \lambda_{i-1}^{m} \]

\[ - \lambda_{i}^{m} \Delta t \lambda_{i}^{m} + \left[ \frac{D_\ell \Delta t}{2(\Delta z)^2} - \lambda_{i}^{m} \frac{\Delta t}{2\Delta z} \right] \lambda_{i}^{m} \lambda_{i-1}^{m} \Delta t \]

Let

\[ \lambda_{A_i} = \frac{D_\ell \Delta t}{2(\Delta z)^2} \]

\[ \lambda_{B_i} = 1 + \frac{D_\ell \Delta t}{(\Delta z)^2} \]

\[ = 1 + 2\lambda_{A_i} \]

\[ \lambda_{C_i}^{m} = \left[ \frac{D_\ell \Delta t}{2(\Delta z)^2} + \lambda_{i}^{m} \frac{\Delta t}{2\Delta z} \right] \lambda_{i}^{m} + \left[ 1 - \frac{D_\ell \Delta t}{(\Delta z)^2} - \lambda_{i}^{m} \Delta t \right] \lambda_{i}^{m} \]

\[ + \left[ \frac{D_\ell \Delta t}{2(\Delta z)^2} - \lambda_{i}^{m} \frac{\Delta t}{2\Delta z} \right] \lambda_{i}^{m} \lambda_{i-1}^{m} \Delta t \]

Thus equation (A3-13) becomes

\[ -\lambda_{A_i}^{i+1} \lambda_{i}^{m+1} + \lambda_{B_i} \lambda_{i}^{m} + \lambda_{A_i} \lambda_{i-1}^{m} \lambda_{i}^{m+1} = \lambda_{C_i}^{m} \]
The boundary conditions are

\[
\begin{align*}
\ell = 1 & \quad \ell \phi_i^1 = 0 \quad \text{for all } i \\
\ell = 1 & \quad \ell \varphi_i^m = 0 \quad \text{for all } i \\
\ell = L & \quad \ell \varphi_i^m - \ell^{-1} \varphi_i^n = 0 \quad \text{for all } i \\
\end{align*}
\]  

(A3-18)
APPENDIX IV

COMPUTER PROGRAM LISTINGS

BOLTSOL

C THIS PROGRAM CALCULATES THE
C VIBRATIONAL TEMPERATURE, AND NUMBER DENSITY
C OF VIBRATIONAL QUANTA PRODUCED BY SLOW ELECTRON
C COLLISIONS FOR VIBRATIONAL NITROGEN.
C THE SYMBOLOGY IS THAT CONTAINED IN THE ANALYTICAL
C FORMULATION OF THE PROBLEM.
C THE DIMENSIONS OF PSI WILL CHANGE WITH THE UPPER ALTITUDE
C LIMIT,ZUPPER,THE STEP SIZE,DELZ.
C TIMEX IS THE MAXIMUM TIME AND DELT IS THE TIME STEP.
C PSI SHOULD BE DIMENSIONED ACCORDING TO PSI(IALT, 2 ) WHERE
C MINIMUM VALUE OF IALT IS
C IALT = 1. + (ZUPPER - 120.)/DELZ
C IPMOVE IS (ARRAY SIZE)*BYTES*(NUMBER OF ARRAYS).
C ALL OTHER ARRAYS ARE DIMENSIONED FOR A 10. KM. DELZ.
C MMNTIN GOVERNS THE PRINTER LISTING AND PLOTTING FREQUENCY.
C TCHANG IS THE TIME AT WHICH THE STEP SIZE IS CHANGED
C TO DELT2 FROM DELT.
C ITFLAG IS A FLAG TO INDICATE TO THE PROGRAM THAT MORE
C THAN ONE TIME STEP IS USED.
C IFLAG IS RELATED TO ITFLAG AND IS INITIALLY SET TO ZERO.
C ICFLAG IS A FLAG TO INDICATE TO THE PROGRAM THAT A CORRECTION
C USING RESULTS FROM PROGRAM BOLTDEV IS TO BE APPLIED TO
C THE SOURCE TERM OF THIS PROGRAM.

REAL *4 NED,NI,INT,N2,NE,MBAR,N2Z,NZ1,NZ2,MBAR1,MBAR2,NOZ
LOGICAL*1 IMAGE(5151)
DIMENSION RAID(8),TED(80),ZD(10),NED(45)
C ,GAMIZD(70),X1(15),Y1(15),ZP(15)
C ,ID1(15),IDZ(15),Z(89),NOZ(89),KATEOE(89),KATEOD(89)
C ,TEI(2),TE(89),NZ(6),NE(89),A(89)
C ,NZ1(6),NZ2(6),P1(6,6),P2(6,6),P3(6,6),P4(6,6)
C ,INT(6,6),E(10),B(89),C(89),D1(89),D2(89)
C ,D3(89),
C ,D8(89),D1I(89),PSI(89,2)
C ,EC(89),F(89),TV(90),QUANT(89),N2I(89)
C ,TZZI(89),
C ,ALPSI(90),GRID(8281),CORR(89)
C ,ALN2Z(89),ALN89),ALNE(89),A
C ,ALQUAN(89),DSOUR(89),DSOURC(89),TV(1)
C ,PHI(6,21),EPSIL(6,21),N8OLT(6,21),SUMC(6,6),G1(1),N2Z1(1)
C DATA INPUT.
READ (5,1,END=90000) KAIL
1 FORMAT (F5,1)
WRITE (6,2)KAIL
2 FORMAT (*1,8F6,1)
READ (5,3,END=90000) TED
3 FORMAT (F6,0)
WRITE (6,4) TED
4 FORMAT (*0,10F7,0)

128
READ (5,5,END=90000) ZD
5 FORMAT (F5.0) ZD
WRITE (6,6) ZD
6 FORMAT ('O',10F6.0)
READ (5,7,END=90000) NED
7 FORMAT (E13.7)
WRITE (6,8) NED
8 FORMAT ('O',10E12.5)
READ (5,10,END=90000) GAMIZD
10 FORMAT (E13.7)
WRITE (6,11) GAMIZD
11 FORMAT ('O',8E14.7)
READ (5,12,END=90000) DELZ,ZUPPER,DELT,TIMEX,MMMTIN,ITFLAG
12 FORMAT (F4.0,F5.0,F6.0,F7.0,F7.0,F6.0,F6.0,F12,E10.2)
WRITE (6,13) DELZ,ZUPPER,DELT,TIMEX,MMMTIN,ITFLAG,TCHANG,DEL2,
13 FORMAT (F6.4,F6.0,E13.7,F5.3,F5.0)
WRITE (6,15) DII,TI,NI,ENU,RAI
15 FORMAT ('O',1X,F6.4)
WRITE (6,17) E
17 FORMAT ('O',10(I1X,F6.4))
READ (5,18,END=90000) (W(N),X(N),Y(N),ZP(N),
18 FORMAT (1X,4E14.6,3X,2I1)
WRITE (5,20,END=90000) RAI
20 FORMAT (F5.1)
WRITE (6,21) RAI
21 FORMAT ('O',F5.1)
C RECONSTRUCTION OF THE INTEGRATED CHEN CROSS-SECTIONS
C PARAMETERS.
WRITE (6,26)
26 FORMAT ('O',2X,'ID',2X,'III',2X,'JJJ',8X,'P1',9X,'P2',
27 FORMAT ('O',13X,'P3',12X,'P4')
DO 2700 IM=1,15
27 FORMAT (1X,4E14.6,3X,2I1)
DO 2700 IM=1,15
II = ID1(IM) + 1
JJJ = ID2(IM) + 1
P1(III,JJJ) = W(IM)
P2(III,JJJ) = X(IM),
P3(III,JJJ) = Y(I)
P4(III,JJJ) = Z(I)

2700 WRITE (6,27) I01(I),I02(I),III,JJJ,P1(III,JJJ)
   +P2(III,JJJ),P3(III,JJJ),P4(III,JJJ)
27 FORMAT ('1*1,2X,'II,3X,'III,JJJ,M14.6)  
C TEST OF RAI FOR TABLE RANGE.
   DO 2100 I=1,7
   II = I
2100 IF (RAI.GE.RAI(I).AND.RAI.LT.RAI(I+1)) GO TO 2300
   WRITE (6,22)
22 FORMAT ('1*1,RAI NOT WITHIN TABLE RANGE*')
   WRITE (6,23) RAI
   STOP
2300 CONTINUE
C SET DIAGONAL ELEMENTS OF INTEGRATED CROSS-SECTION MATRIX
C TO ZERO.
   DO 2900 IIK=1,6
   INT(IIK,IIK) = 0.
   IFLAG = 0
   MLow = 2
   BK = 8.61703E-05
   THETA = 3380.  
   MMAX = TCHANG/DELT
   MMIN = 0
   DIFI = (DI+NI)/(NI*0.75)
   CALL JACH2 (Z,TOO,TZ,NZtBAR,RHOZ,HZ)
C CALCULATION OF TIME INVARIANT COEFFICIENTS AT EACH
C VERTICAL GRID POINT.
   LMAX = 1 + (ZUPPER - 120.)/DELZ
3900 WRITE (6,41)
   41 FORMAT ('1*1,5X,'DIFF',10X,'A',12X,'H',12X,'C',12X,
   +C 'D1',12X,'D2',10X,'D3', 5X,'L')
   DO 2000 L=1,LMAX
      Z(L) = 120. + (L -1)*DELZ
C TEST OF Z TO BE WITHIN TABLE RANGES.
   DO 2400 K=1,9
2400 IF (Z(L).GE.ZD(K).AND.Z(L).LT.ZD(K+1)) GO TO 2500
   WRITE (6,24)
24 FORMAT ('1*1,ALTITUDE IS NOT WITHIN TABLE RANGE*')
   WRITE (6,25) Z(L)
   STOP
2500 IK = K
IL = K + 1

C CALCULATION OF TEI.
C TEI INDEX IS THE LINE NUMBER.
C OF THE PLOTTED ELECTRON TEMPERATURE DATA.
DO 2600 LL=1,2
2600 TEI(LL) = GANIZD(IK + 10*(II-1) + LL - 1)
C = RAI - RAID(II) + TED((II-1)*10 +IK+LL-1)

C CALCULATION OF BETAZI AND THE ELECTRON TEMPERATURE.
BETAZI = (TEI(2) - TEI(1))/(ZD(IL) - ZD(IK))
TE(L) = BETAZI*(Z(L) - ZD(IK)) + TEI(1)

C CALCULATION OF ELECTRON DENSITY.
DO 100 IT=1,44
ZTEST1 = 20.*(IT-1) + 120.
ZTEST2 = ZTEST1 + 20.
IF ( Z(L).GE.ZTEST1.AND.Z(L).LE.ZTEST2) GO TO 200
100 CONTINUE
WRITE (6,51) 0
51 FORMAT ('0','ALTITUDE FOR NE CALCULATION IS OUTSIDE TABLE')
WRITE (6,52) Z(L)
52 FORMAT ('0',2X,F6.0)
STOP

200 ITT = IT
GRADNE = (NED(ITT+1) - NED(ITT))/20.
NE(L) = GRADNE*(Z(L) - ZTEST1) + NED(ITT)
ZA = Z(L)
CALL JACH2(ZA,TOO,TZ,NZ,M8AR,RHOZ,HZ)
N2Z(L) = NZ(1)
NOZ(L) = NZ(3)
SUMNZ = NZ(1) + NZ(3)
TZZ(L) = TZ
RATEOD(L) = RATEOD(L)*EXP(-THETA/TZZ(L))

C CALCULATION OF DIFFUSION, A AND B COEFFICIENTS.
DIFF = DIFI*(TZ*0.75)/SUMNZ
A(L) = (DIFF * DELT)/(2. *(((DELZ+1.)*E+05)**2.))
B(L) = 1. + 2.*A(L)
IF(L.EQ.1) GO TO 200

C CALCULATION OF DERIVATIVE OF PRODUCT OF DIFFUSION
C COEFFICIENT AND MOLECULAR NITROGEN DENSITY
C WITH RESPECT TO ALTITUDE.
Z1 = Z(L) - 0.5*DELZ
Z2 = Z(L) + 0.5*DELZ
CALL JACH2(Z1,TOO,TZ1,NZ1,M8AR,RHOZ1,HZ1)
CALL JACH2(Z2,TOO,TZ2,NZ2,M8AR2,RHOZ2,HZ2)
SUMNZ1 = NZ1(1) + NZ1(3)
SUMNZ2 = NZ2(1) + NZ2(3)
DIFF1 = DIFF1*(TZ1**0.75)/SUMNZ1
DIFF2 = DIFF2*(TZ2**0.75)/SUMNZ2
DERIV = (DIFF2*NZ2(1) - DIFF1*NZ1(1))/(DELT*1.E+05)

C CALCULATION OF C AND TIME INDEPENDENT PARTIAL D COEFFICIENTS.
C(L) = (DERIV*DELT)/(2.*(DELT*1.E+05)*NZ1(1))
D1(L) = A(L) + C(L)
D2(L) = 1. - 2.*A(L)
D3(L) = A(L) - C(L)

WRITE (6,42) DIFF, A(L), B(L), C(L), D1(L), D2(L), D3(L), L
42 FORMAT ('O',1P7E13.5,1I3)

2000 CONTINUE
C(1) = C(2)
D1(1) = A(1) + C(1)
D2(1) = 1. - 2.*A(1)
D3(1) = A(1) - C(1)

61 FORMAT ('1',2X,'ALT',6X,'RATEOE',8X,'RATEOD',5X,'N(O)')
WRITE (6,61) 00019301
61 FORMAT ('0',OPF5.0,1P3E13.5)

IF (IFLAG.EQ.1) GO TO 3950

C CALCULATION OF EC AND F COEFFICIENTS FOR INITIAL TIME STEP.
C LLL IS THE ALTITUDE STEP INDEX.
EC(1) = 0.
F(1) = 7.329241E-05

WRITE (6,43) 00020000
43 FORMAT ('1',6X,'DI',1OX,'EC',1OX,'F',1OX,'DENOM',1OX,'LLL')

DO 3200 LLL=1,LMAX
C SET DSOURC TO ZERO.
DSOURC(LLL) = 0.

C CALCULATION OF INTEGRATED CHEN CROSS-SECTION VALUES
BkTEE = BK*TE(LLL)
RTE = 1./TE(LLL)
RTE2 = RTE*RTE
RTE3 = RTE2*RTE

DO 2800 IN=1,15
IIJ = ID1(IN) + 1
JJJ = ID2(IN) + 1
INT (IIJ,JJJ) = EXP(P1(IIJ,JJJ) + P2(IIJ,JJJ)*RTE + P3(IIJ,JJJ)*RTE2 + P4(IIJ,JJJ)*RTE3)

2800 INT(JJJ,IIJ) = INT(IIJ,JJJ)*EXP(-E(JJJ) - E(IIJ))/BKTEE

C CALCULATION OF INITIAL SOURCE TERM DI.
SUMSI = 0.
DO 3400 IIL = 1,6

4000 CONTINUE

SUM = (IIL - 1) * INT(IIL, 1) * NE(LLL)
SUMSI = SUMSI + SUM
DI(LLL) = SUMSI * DELT + RATEOE(LLL) * DELT * (F(1) + 1. -
   F(1) * EXP(THETA/TZZ(LLL)))
C END CALCULATION OF INITIAL SOURCE TERM AT ALTITUDE DENOTED BY LLL.
IF (LLL .EQ. 1) GO TO 3200
DENOM = B(LLL) - A(LLL) * EC(LLL - 1)
EC(LLL) = A(LLL) / DENOM
DI(LLL) = (DI(LLL) + A(LLL) * F(LLL - 1)) / DENOM
WRITE (6, 44) DI(LLL), EC(LLL), F(LLL), DENOM, LLL
44 FORMAT ('O', 1P4E13.6, I3)
3200 CONTINUE
C CALCULATION OF INITIAL PSI.
MMM = 1
LLMAX = LMAX - 1
PSI(LLMAX - 1, 1) = F(LLMAX - 1) / (1. - EC(LLMAX - 1))
DO 3500 NNN = 2, LLMAX
   MMMM = LMAX - NNN
   PSI(NNNM, 1) = EC(NNNM) * PSI(NNNM + 1, 1) + F(NNNM)
   NNNN = NNN + 1
   TV(NNNN) = THETA / ALOG((PSI(NNNN) + 1.) / PSI(NNNN, 1))
   QUANTA(NNNN) = N2Z(NNNN) * PSI(NNNN, 1)
3500 CONTINUE
PSI(LMAX, 1) = PSI(LMAX - 1, 1)
PSI(LMAX + 1, 1) = PSI(LMAX, 1)
TV(LMAX) = THETA / ALOG((PSI(LMAX + 1, 1) + 1.) / PSI(LMAX, 1))
TV(1) = 0.
QUANTA(1) = 0.
QUANTA(LMAX) = N2Z(LMAX) * PSI(LMAX, 1)
C WRITE RESULTS ON OUTPUT TAPE.
WRITE (10) (Z(ILN), TV(ILN), NE(ILN), QUANTA(ILN), PSI(ILN, 1), DI(ILN),
   DELZ, MMM, DELT, IFLAG, ICFLAG, MMMIN)
WRITE (6, 34) MMM, MMM, MMM, MMM, MMM, MMM, MMM, MMM
34 FORMAT ('O', 1P4F5.0, 2X, 'TV', 1P8E13.5)
35 FORMAT ('O', 1P4F5.0, 2X, 'TV', 1P8E13.5)
C WRITE RESULTS ON OUTPUT TAPE FOR OTHER TIME STEPS.
WRITE (10) (Z(IKN), TV(IKN), NE(IKN), QUANTA(IKN), PSI(IKN, 1), DI(IKN),
   DELZ, MMM, DELT, IFLAG, ICFLAG, MMMIN)
WRITE (6, 28) (Z(IKN), TV(IKN), NE(IKN), QUANTA(IKN), PSI(IKN, 1), DI(IKN),
   DELZ, MMM, DELT, IFLAG, ICFLAG, MMMIN)
28 FORMAT ('O', 1P4F5.0, 2X, 'TV', 1P8E13.5)
C MMT IS AN INDEX CONTROLLING THE AMOUNT OF PRINTED OUTPUT.
C MMM IS THE TIME STEP INDEX.

    MMT = 2
    IF (ICFLAG.EQ.0) GO TO 3950
    READ (11,END=90001,ERR=90002) MMIN,DELT1,LBOUND,DELZ1,DELZ2,
    X LINC,(G(I),N2ZI(I),TV1(I),I,PHI(I),ILN),EPSIL(I),ILN),
    X NBOLT(I,ILN),I=1,6,1,ILN=1,LMAX)

3950 DO 3600 MMM=MLOW,MMAX
    DO 3700 LLLL=1,LMAX
      IF (LLLL.EQ.1) D(1)=D1(1)*PSI(2, 1 )+DI(1)
      IF (LLLL.EQ.1) GO TO 3700
      C CALCULATION OF INTEGRATED CHEN CROSS-SECTION VALUES
      AT ALTITUDE OF INTEREST.
      BKTE = BK*TE(LLLL)
      RTE = 1./TE(LLLL)
      RTE2 = RTE*RTE
      RTE3 = RTE2*RTE
      DO 3801 IJK=1,15
         INI = ID1(IJK) + 1
         INJ = ID2(IJK) + 1
         INT(INI,INJ) = EXP(P1(INI,INJ) + P2(INI,INJ)*RTE
         C + P3(INI,INJ)*RTE2 + P4(INI,INJ)*RTE3)
      3801 INT(INJ,INI) = INT(INI,INJ)*EXP(-(E(INJ)
         - E(INI))/BKTE)
      C CALCULATION OF D COEFFICIENT AT ALTITUDE LLLL.
      SUMST = 0.
      DO 3901 IIII=1,6
         DO 3901 JJJJ=1,6
            SUMS = 1./(PSI(LLLL, 1 ) + 1.)*((PSI(LLLL, 1 )/ 0002
            C (PSI(LLLL, 1 )+1.))**(JJJJ-1))*(IIII-JJJJ)
         3901 SUMST = SUMST + SUMS
      IF (ICFLAG.EQ.0) GO TO 1500
1100 IF(MMM-MMIN)1500,1200,90003
1200 SUMT = 0.
   DO 1300 II=1,6
      DO 1300 JJ=1,6
         SUMC(II,JJ) = INT(II,JJ)*NE(LLLL)*EPSIL(JJ,LLLL)*(II-JJ)
1300 SUMT = SUMT + SUMC(II,JJ)
   CORR(LLLL) = SUMT/N2ZI(LLLL)
   DSOURC(LLLL) = CORR(LLLL)*DELT
   IF (LLLL.EQ.LMAX) GO TO 1000
   GO TO 1600
1000 READ (11,END=90001,ERR=90002) MMIN,DELT1,LBOUND,DELZ1,DELZ2,
   X LINC,(G(I),N2ZI(I),TV1(I),I,PHI(I),ILN),EPSIL(I),ILN),
   X NBOLT(I,ILN),I=1,6,1,ILN=1,LMAX)
GO TO 1600
1500 DSOURC(LLLL) = 0.
1600 CONTINUE
DSOURC(LLLL) = SUMST*DELT + DSOURC(LLLL)
DILLL = D1(LLLL)*PSI(LLLL+1, 1 ) + D2(LLLL)*PSI(LLLL, 1 )
C + D3(LLLL)*PSI(LLLL-1, 1 ) + DSOURC(LLLL)
X + RATEOE(LLLL)*DELT*(PSI(LLLL,1) + 1) + X - PSI(LLLL+1)*EXP(THETA/TZZ(LLLL)))
DENOM1 = B(LLLL) - A(LLLL)*EC(LLLL-1)
EC(LLLL) = A(LLLL)/DENOM1
F(LLLL) = (D(LLLL) + A(LLLL)*F(LLLL-1))/DENOM1
3700 CONTINUE
C CALCULATION OF PSI, VIBRATIONAL TEMPERATURE, ETC.
PSI(LMAX-1, 2 ) = F(LMAX-1)/(1.-EC(LMAX-1))
PSI(LMAX, 2 ) = PSI(LMAX-1, 2 )
DO 4000 INN=2,LMAX
NNNNN = LMAX - INN
PSI(NNNNN, 2 ) = EC(NNNNN)*PSI(NNNNN+1, 2 ) + F(NNNNN)
NnNNN = NNNNN + 1
TV(NNNNNM) = THETA/ALOG((PSI(NNNNNM, 2 )+1.)/PSI(NNNNNM, 2 ))
4000 QUANTA(NNNNNM) = N2Z(NNNNNM)*PSI(NNNNNM, 2 )
TV(LMAX ) = THETA/ALOG((PSI(LMAX , 2 )+1.)/PSI(LMAX , 2 ))
TV(1) = 0.
QUANTA(1) = 0.
QUANTA(LMAX ) = N2Z(LMAX )*PSI(LMAX , 2 )
C WRITE RESULTS ON OUTPUT TAPE.
WRITE (10) (Z(ILN),TZZ(ILN),TE(ILN),TV(ILN),N2Z(ILN),NE(ILN),
C QUANTA(ILN),PSI(ILN, 2 ),DI(ILN),D(ILN),DSOUR(ILN),
C DSOURC(ILN),ILN=1,LMAX)
WRITE (6,29)
29 FORMAT ('1',46X,'TEMPERATURES VERSUS ALTITUDE')
   XR = 1000.
   XL = 0.
   YT = 10000.
   YB = 0.
   NUMPR1 = LMAX + 1
   NUMPR2 = LMAX
   CALL PLOT2 (GRID,XR,XL,YT,YB)
   CALL PLOT3 ('T',Z,TZ,NUMPR1)
   CALL PLOT3 ('V',Z,TV,NUMPR1)
   CALL PLOT4 (20,'TEMPERATURE DEG. K')
   WRITE (6,30)
30 FORMAT ('0',59X,'ALTITUDE (KM.)')
   WRITE (6,31)
31 FORMAT ('1',51X,'PSI VERSUS ALTITUDE')
   YT = 0.0
   YB = -5.0
   CALL PLOT2 (GRID,XR,XL,YT,YB)
   CALL PLOT3 ('*',Z,ALPSI,NUMPR2)
   CALL PLOT4 (3,'PSI')
   WRITE (6,30)
   YT = +9.0
   YB = +4.0
   WRITE (6,32)
32 FORMAT ('1',46X,'QUANTA AND ELECTRON DENSITIES')
   CALL PLOT2 (GRID,XR,XL,YT,YB)
   CALL PLOT3 ('E',Z,ALNE,NUMPR2)
   CALL PLOT3 ('Q',Z,ALOUAN,NUMPR2)
   CALL PLOT4 (23,'NUMBER DENSITY CM**-3')
   WRITE (6,30)
3600 CALL CMOVE(IPMOVE,PSI(1,2),1,PSI(1,1),1)
   CONTINUE
C TEST FOR CHANGE OF TIME STEP.
   MLOW = MMAX + 1
   IF (ITFLAG.EQ.1.AND.IFLAG.EQ.0) GO TO 3800
   END FILE 10
   STOP
C SET UP DO LOOP INDICES FOR SECOND TIME INCREMENT STEP SIZE.
3800 DELT = DELT2
   MMAX = (TIMEX - TCHANG)/DELT2 + MLOW - 1
   IFLAG = ITFLAG
   GO TO 3900
90000 WRITE (6,33)
33 FORMAT ('1','END OF FILE ENCOUNTERED ON CARD READER')
STOP
90001 WRITE (6,84)
   84 FORMAT ('1', 'END OF FILE ENCOUNTERED ON INPUT TAPE')
   STOP
90002 WRITE (6,85)
   85 FORMAT ('1', 'IO ERROR ENCOUNTERED ON INPUT TAPE')
   STOP
90003 WRITE (6,86)
   86 FORMAT ('1', 'MMIN IS LESS THAN MMM')
   STOP
END

REAL *4 NED,NI,INT,NZ,NE,MBAR,N2Z,NZ1,NZ2,MBAR1,MBAR2,NU,NBOLT,NOZ
INTEGER TINC,TINC2
LOGICAL*1 IMAGE(5151)
DIMENSION Z(89),RAID(8),TED(80),ZD(10),NED(45)
X ,NZ(6),NE(89),A(89),NOZ(89)
X ,W(15),X(15),Y(15),ZP(15),ID1(15)
X ,ID2(15),TEI(2),TE(89),P1(6,6)
X ,P2(6,6),P3(6,6),P4(6,6),INT(6,6)
X ,N1(6),N2(6),GRAD(89),HPRESS(89)
X ,E(10),R(89),MBAR1(3),DELT1(3),IFLAG(3),
X ,NZ(89), MM(3),D1(89),PSI(30,3),KATE0(89),KATE0(89)
X ,TZZ(89),GRID(8281),SUM1A(89),SUM2A(89)
X ,DERIVD(89),DIFF(89),H(89),DPSIZ(89),DPSIT(89)
X ,DPSIZ(89),ALPHA(6,89),BETA(6,89),GAMMA(6,89)
X ,NU(89),P1001(89),TV(30,3),QUANTA(30,1),D(30,1)
X ,PHI(6,89),C1(6,89),C2(6,89),C3(6,89),C4(6,89),F(6,89)
X ,EC(6,89),ALPHI1(89),ALPHI2(89),ALPHI3(89),ALPHI4(89),
X ALPHI5(89),ALPHI6(89),EPSIL(6,89),NBOLT(6,89),REPSIL(6,89)
C DATA INPUT.
READ (5,1,END=90000) RAID
1 FORMAT (F5.1)
WRITE (6,2) RAID
2 FORMAT ('1',BF5.1)
READ (5,3,END=90000) TED
3 FORMAT (F6.0)
WRITE (6,4) TED
4 FORMAT ('0',10F7.0)
READ (5,5,END=90000) ZD
5 FORMAT (F5.0)
WRITE (6,6) ZD
6 FORMAT ('0',10F7.0)
READ (5,7,END=90000) NED
7 FORMAT (E11.5)
WRITE (6,8) NED
8 FORMAT ('0',10E12.5)
READ (5,10,END=90000) GAMIZD
10 FORMAT (E13.7)
WRITE (6,11) GAMIZD
11 FORMAT ('0',8E14.7)
READ (5,12,END=90000) DELZ,ZUPPER,DELT,TIMEX,MMMTIN,LINC,TINC
12 FORMAT ('0',14,4E10.2)
X ,LBOUND,TINC2,RATED
13 FORMAT ('0',F4.0,F5.0,F6.0,F7.0,F8.0,F9.0,F10.0,F11.0,F12.0)
READ (5,14,END=90000) D11,T1,N1,ENU,T00
14 FORMAT (F5.0,F6.0,F7.0,F8.0,F9.0,F10.0,F11.0,F12.0)
WRITE (6,15) D11,T1,N1,ENU,T00
15 FORMAT ('0',F5.0,F6.0,F7.0,F8.0,F9.0,F10.0,F11.0,F12.0)
READ (5,16,END=90000) E
16 FORMAT ('0',F5.0,F6.0,F7.0,F8.0,F9.0,F10.0,F11.0,F12.0)
WRITE (6,17) E
17 FORMAT ('0',10E15.7)
READ (5,18,END=90000) (W(N),X(N),Y(N),ZP(N),
18 FORMAT ('0',10X,F6.4))
WRITE (6,19) (W(N),X(N),Y(N),ZP(N),ID1(N),ID2(N),N=1,15)
C
19 FORMAT ('0',10X,F6.4)
WRITE (6,20) (W(N),X(N),Y(N),ZP(N),ID1(N),ID2(N),N=1,15)
20 FORMAT (F5.1)
WRITE (6,21) RAI
21 FORMAT ('0',F5.1)
READ (5,22) ISTART
C RECONSTRUCTION OF THE INTEGRATED CHEN CROSS-SECTIONS
C
WRITE (6,26)

DO 2700 IM=1,15
   III = ID1( IM ) + 1
   JJJ = ID2( IM ) + 1
   P1(III,JJJ) = W( IM )
   P2(III,JJJ) = X( IM )
   P3(III,JJJ) = Y( IM )
   P4(III,JJJ) = ZP( IM )

2700 WRITE (6,27) ID1(IM),ID2(IM),III,JJJ,P1(III,JJJ),P2(III,JJJ),P3(III,JJJ),P4(III,JJJ)

C IPMOV AND IMMOV ARE (ARRAY SIZE)*BYTES*(NUMBER OF ARRAYS)
IPMOV = 30**4*2
IMMOV = 1*4*2
BK = 8.61703E-05
THETA = 3380.

ISTAR = ISTART - 1
LMAX = 1. + (ZUPPER - 120.)/DELZ

C SET PHI(I,L),EC(I,LBOUND),AND F(I,LBOUND) TO ZERO.
C SET REPSIL(I,LBOUND) AND DIAGONAL ELEMENTS OF THE
C INTEGRATED CHEN CROSS-SECTION MATRIX TO ZERO.

DO 3000 IJ = 1,6
   DO 3001 K=1,LBOUND
      EC(IJ,K) = 0.
      F(IJ,K) = 0.
      REPSIL(IJ,LBOUND) = 0.
      INT(IJ,IJ) = 0.
   3001 PHI(IJ,K) = 0.
   DO 3000 LL = 1,LMAX,LINC
3000 PHI(IJ,LL) = 0.

C READ TAPE CONTAINING BOLTZMAN PART SOLUTION.
READ ( 10,END=90001,EKR=90002) (Z(ILN),TZZ(ILN),TE(ILN),
   TV(ILN,1),N2Z(ILN),NE(ILN),QUANTA(ILN,1),
   PSI(ILN,1),DI(ILN),O(ILN,1),MAM(1),DELZ1,
   NMAX(1),DELT1,1,IFLAG(1),ILN=1,LMAX)

IF (ISTAR - MAM(1)) 90003,3600,4100
3600 DO 3700 %=2,3
3700 READ (10,END=90001,ERR=90002) (Z(ILN),TZ(ILN),TE(ILN),
  X TV(ILN,M),N2Z(ILN),NE(ILN),QUANTA(ILN,1),
  X PSI(ILN,M),DI(ILN),D(ILN),MMM(M),DELZ1,
  X MMAX1(M),DELT1(M),IFLAG(M),ILN=1,LMAX)
  MMT = ISTAR + 1
  GO TO 6000
  4100 DO 1000 JK=3,ISTAR
  1000 READ (10,END=90001,ERR=90002)
  MMT = ISTART + 1
  DO 4200 LM=1,3
  4200 READ (10,END=90001,ERR=90002)
  3900 DO 3901 J=1,TINC
  CALL CMOVE (IPMOV,PSI(1,2),1,PSI(1,1),1)
  CALL CMOVE (IPMOV,TV(1,2),1,TV(1,1),1)
  CALL CMOVE(IMMOV,MMM(2),1,MMM(1),1)
  CALL CMOVE(IMMOV,DELT(2),1,DELT(1),1)
  CALL CMOVE(IMMOV,IFLAG(2),1,IFLAG(1),1)
  READ (10,END=90001,ERR=90002)
  MMT = ISTART + 1
  DO 4200 LM=1,3
  4200 READ (10,END=90001,ERR=90002)
  MMT = ISTART + 1
  GO TO 6000
  3900 DO 3901 J=1,TINC
  CALL CMOVE (IPMOV,PSI(1,2),1,PSI(1,1),1)
  CALL CMOVE (IPMOV,TV(1,2),1,TV(1,1),1)
  CALL CMOVE(IMMOV,MMM(2),1,MMM(1),1)
  CALL CMOVE(IMMOV,DELT(2),1,DELT(1),1)
  CALL CMOVE(IMMOV,IFLAG(2),1,IFLAG(1),1)
  READ (10,END=90001,ERR=90002)
  MMT = ISTART + 1
  GO TO 6000
  3901 CONTINUE
  GO TO 3800
  C CALCULATION OF A,B AND OTHER TIME INVARIANT TERMS.
  6000 DELT = DELT(1)
  IF (IFLAG(3).EQ.1) TINC = TINC2
  EDEL = DELT*TINC
  DO 2500 II=1,LMAX,LINC
  CALL JACH2 (Z(II),TOO,TZ,NZ,MBAR,RHOZ,HZ)
  HPRESS(II) = HZ*MBAR/28.
  NOZ(II) = NZ(3)
  SUMNZ = NZ(1) + NZ(3)
  DIFF(II) = DIFI*(TZ**0.75)/SUMNZ
  AI(II) = (DIFF(II)*EDEL)/(2.*((DELZ*LINC*1,E+05)**2.))
  BI(II) = 1. + 2*A(II)
  T05 = TZ**0.5
  NU(II) = 1.48209*1E-11*T05
  P1001(II) = 2.6003E-06*TZ*EXP(91.5/TZ)
  RATEOD(II) = RATE0*NU(II)
RATEOE(II) = RATEOD(II) * EXP(-THETA/TZZ(I)) 142

C CALCULATION OF DERIVATIVES OF DIFF., TEMP., AND DENSITY SCALE HEIGHT.

IF (II.EQ.1) GO.TO 2500
Z1 = Z(II) - 0.5*DELZ
Z2 = Z(II) + 0.5*DELZ
CALL JACH2(Z1, TOO, TZ1, NZ1, MBAR1, KHOZ1, HZ1)
CALL JACH2(Z2, TOO, TZ2, NZ2, MBAR2, KHOZ2, HZ2)
GRADT(II) = (TZ2 - TZ1)/DELZ
H(II) = HPRESS(II)/(1 + HPRESS(II) * GRADT(II)/TZZ(II))
SUMNZ1 = NZ1(1) + NZ1(3)
SUMNZ2 = NZ2(1) + NZ2(3)
DIFF1 = DIFI*(TZ1**0.75)/SUMNZ1
DIFF2 = DIFI*(TZ2**0.75)/SUMNZ2
DERIVD(II) = (DIFF2 - DIFF1)/(DELZ*1.E+05) 2500 CONTINUE

GRADT(1) = GRADT(2)
H(1) = HPRESS(1)/(1 + HPRESS(1) * GRADT(1)/TZZ(1))
DERIVD(1) = DERIVD(2)
LINC1 = LINC + LBOUND
LLMAX = LMAX - LINC
MMMAX = MMAX(3) - 1

3800 DO 4000 L = LINC1, LLMAX, LINC

C CALCULATION OF DERIVATIVES OF PSI WITH RESPECT TO ALTITUDE AND TIME.

DPSIZ(L) = (PSI(L+1,2) - PSI(L-1,2))/(2*(DELZ*1.E+05))
D2PSIZ(L) = (PSI(L+1,2) - 2*PSI(L,2) + PSI(L-1,2))/(DELZ**2)
DELTS = DELT1(1) + DELT1(3)
DPSIT(L) = (PSI(L,3) - PSI(L,1))/(2*DELTS)

C CALCULATION OF INTEGRATED CHEN CROSS-SECTION VALUES AT ALTITUDE OF INTEREST.

BKTE = BK*TE(L)
RTE = 1./TE(L)
RTE2 = RTE*RTE
RTE3 = RTE2*RTE
DO 2800 IN = 1, 15
IIJ = ID1(IN) + 1
JJJ = ID2(IN) + 1
INT(IIJ, JJJ) = EXP(P1(IIJ, JJJ) + P2(IIJ, JJJ)*RTE + P3(IIJ, JJJ)*RTE2 + P4(IIJ, JJJ)*RTE3) 2800 CONTINUE

BRAKET = (1-1)/PSI(L,2) - 1/(PSI(L,2) + 1.)
ALPHA(1, L) = DERIVD(L) + DIFF(L)*(-E(JJJ) - E(IIJ))/BKTE
X = DPSIZ(L))
C CALCULATION OF SOURCE TERMS.
C CALCULATION OF SUMMATIONS FOR USE IN BETA AND GAMMA.

SUM1 = 0.
SUM2 = 0.
DO 5000 IIL=1,6
  SUM1 = INT(IIL)*NE(L)
  SUM2 = SUM1 + INT(IIL)*NE(L)
  SUM1 = SUM1 + PHI(IIL,L)*EXP((1 - IIL)*THETA/TV(L,2))
      SUM2 = SUM2 + PHI(IIL,L)*EXP((1 - IIL)*THETA/TV(L,2))
  5000 SUM2 = SUM2 + SUM1

BETA(I,L) = BKRAKET*DPSIT(L) - DPSIZ(L) + BRAKET*(DERIVD(L) +
          PHI(I-1,L,L)*EXP(-THETA/TV(L,2))*PSI(L-1,I)*PHI(I-1,L)
          + RATEOE(L)*PHI(I-1,L)*EXP(THETA/TZZ(L)) +
          I*(PSI(L,2) + 1.))
      GAMMA(I,L) = SUM2 - BETA(I,L)

C CALCULATION OF EC(I,L) AND F(I,L) COEFFICIENTS.

DENOM = B(L) - EC(I,L)*DELZ/LINC
EC(I,L) = A(L) + ALPHA(I,L)*EC1(I,L)*DELZ/LINC
F(I,L) = (EC(I,L) + A(L))*F(I,L)*DELZ/LINC

C CALCULATION OF PHI.
IF (LBOND.EQ.1) GO TO 4300
DO 4301 IL=1,6
NBOLT(IL,LBOND) = N2Z(ILBOUND)*(1./(PSI(LBOUND,2) + 1.))**X((PSI(LBOUND,2)/(PSI(LBOUND,2) + 1.))**(1L - 1))
4301 EPSIL(IL,LBOND) = 0.*
GO TO 4400
4300 NBOLT(1,1) = N2Z(1)
NBOLT(2,1) = 0.*
NBOLT(3,1) = 0.*
NBOLT(4,1) = 0.*
NBOLT(5,1) = 0.*
NBOLT(6,1) = 0.*
EPSIL(1,1) = 0.*
EPSIL(2,1) = 0.*
EPSIL(3,1) = 0.*
EPSIL(4,1) = 0.*
EPSIL(5,1) = 0.*
EPSIL(6,1) = 0.*
4400 DO 4600 IL=1,6
PHI(IL,LLMAX) = F(IL,LLMAX)/(1. - EC(IL,LLMAX))
PHI(IL,LLMAX) = PHI(IL,LLMAX)
NBOLT(IL,LLMAX) = N2Z(LLMAX)*(1./(PSI(LLMAX,2) + 1.))**X((PSI(LLMAX,2)/(PSI(LLMAX,2) + 1.))**(IL-1))
NBOLT(IL,LMAX) = N2Z(LMAX)*(1./(PSI(LMAX,2) + 1.))**X((PSI(LMAX,2)/(PSI(LMAX,2) + 1.))**(IL-1))
EPSIL(IL,LMAX) = PHI(IL,LLMAX)*NBOLT(IL,LLMAX)
EPSIL(IL,LMAX) = PHI(IL,LMAX)*NBOLT(IL,LMAX)
LLLMAX = LMAX - 2*LINC
DO 4700 LL=LINC+1,LMAX,LINC
NN = LMAX - LINC + LBOND - LL
PHI(IL,NN) = EC(IL,NN)*PHI(IL,NN+LINC)+F(IL,NN)
NBOLT(IL,NN) = N2Z(NN)*(1./(PSI(NN,2) + 1.))**X((PSI(NN,2)/(PSI(NN,2) + 1.))**(IL-1))
4700 EPSIL(IL,NN) = PHI(IL,NN)*NBOLT(IL,NN)
CONTINUE
C WRITE RESULTS TO TAPE
WRITE (11) MMM(3),DELT1(3),LBOND,DELZ,DELZ1,LINC,(Z(ILN),X(NZ2(ILN),TV(ILN,2),(I,PHI(I,ILN),EPSIL(I,ILN),X(NBOLT(I,ILN),I=1,6,1),ILN=LBOND,LMAX,LINC)
IF (MMM(2).NE.XRMNT) GO TO 3500
DO 5200 NN=LBOND,LMAX,LINC
SUME1 = 0.*
SUME2 = 0.*
DO 5100 IK=1,6
SUME = EPSIL(1K,NN)
5100 Continue
SUME1 = EPSIL(IK,NN) * (IK-1)
SUME1 = SUME1 + SUME2
5100 SUME2 = SUME2 + SUME1
SUME1A(NN) = SUME1
SUME2A(NN) = SUME2
IF (NN.EQ.0.LBOUND) GO TO 5200
DO 5200 IK=1,6
REPSIL(IK,NN) = SUMEIA(NN)/EPSIL(IK,NN)
5200 CONTINUE

5000 CONTINUE
MMMT = MMMT + MMMTIN
91 FORMAT (11',2X,'C1(I,L)',2X,'C2(I,L)',2X,'C3(I,L)',5X,'C(I,L)', 00025000
X 2X,'GAMMA(I,L)',1X,'ALPHA(I,L)',1X,'BETA(I,L)', 000251000
X 4X,'A(L)',4X,'B(L)',5X,'EC(I,L)',4X,'F(I,L)')
DO 4900 IJK=1,6
WRITE (6,91) 00025600
WRITE (6,92)(C1(IJK,L),C2(IJK,L),C3(IJK,L),C(IJK,L),GAMMA(IJK,L), 00025700
X ALPHA(IJK,L),BETA(IJK,L),A(L),B(L),EC(IJK,L),F(IJK,L), 00025800
X L=LINCP1,LLMAX,LINC)
92 FORMAT (' ',1P11E10.3)
WRITE (6,93)
93 FORMAT ('0',2X,'DPSIT',5X,'DERIVD',4X,'DPSIZ',5X,'D2PSIZ',8X
X ,4X,'H',8X,'P1001',4X,'NU')
WRITE (6,94) (DPSIT(L),DERIVD(L),DPSIZ(L),D2PSIZ(L),H(L),P1001(L),NU(L),L=LINCP1,LLMAX,LINC)
94 FORMAT (' ',1P8E10.3)
WRITE (6,37)
37 FORMAT ('0',2X,'MMM',1X,'LEVEL',3X,'DELTA',3X,'DEDEL')
WRITE (6,35) MMM(3),IJK,DELTA,DEDEL
35 FORMAT ('0',2X,'MM',3X,'IJ',3X,'F5.0',3X,'F5.0')
WRITE (6,34)
34 FORMAT ('0',2X,'ALT',2X,'T',4X,'TV')
X 9X,'(N2)',8X,'PSI',11X,'PHI',8X,'SUM EPSILON', 00025900
X 3X,'SUM EPSILON',3X,'EPSILON',4X,'BOLTZEN',3X,'REPSIL')
4900 WRITE (6,36) (Z(IKN),TZZ(IKN), TV(IKN,2), 00026000
X N2Z(IKN),PSI(IKN,2),PHI(IJK,IKN),SUME1A(IKN), 00026100
X SUME2A(IKN),EPSIL(IJK,IKN),NBOLT(IJK,IKN),REPSIL(IJK,IKN), 00026200
X IKN=LBOUND,LMAX,LINC)
36 FORMAT (' ',OPF5.0,OP2F6.0,1P3E12.3)
C CONSTRUCTION OF PRINTER PLOTTER ARRAYS.
DD 4800 JJ=LBOUND,LMAX
ALPHI1(JJ) = PHI(1,JJ)
ALPHI2(JJ) = PHI(2,JJ)
ALPHI3(JJ) = PHI(3,JJ)
ALPHI4(JJ) = PHI(4,JJ)
ALPHI5(JJ) = PHI(5,JJ)
4800 ALPHI6(JJ) = PHI(6,JJ)
C PRINTER PLOTTING.
   WRITE (6,29).
   29 FORMAT ('1',43X,'DEVIATION VERSUS ALTITUDE')
   XR = 1000.
   XL = 0.
   YT = +14.
   YB = -6.
   NUMPR1 = LMAX + 1
   CALL PLOT2(GRID,XR,XL,YT,YB)
   CALL PLOT3('1',Z,ALPHI1,NUMPR1)
   CALL PLOT3('2',Z,ALPHI2,NUMPR1)
   CALL PLOT3('3',Z,ALPHI3,NUMPR1)
   CALL PLOT3('4',Z,ALPHI4,NUMPR1)
   CALL PLOT3 ('5',Z,ALPHI5,NUMPR1)
   CALL PLOT3 ('6',Z,ALPHI6,NUMPR1)
   CALL PLOT4(3,'PHI')
   WRITE (6,30).
   30 FORMAT ('0',59X,'ALTITUDE (KM.)')
   3500 IF (MMM(2).LT.MMAX) GO TO 3900
   END FILE 11
   STOP
   90000 WRITE (6,33).
   33 FORMAT ('1', 'END OF FILE ENCOUNTERED ON CARD READER')
   STOP
   90001 WRITE (6,84).
   84 FORMAT ('1', 'END OF FILE ENCOUNTERED ON INPUT TAPE')
   STOP
   90002 WRITE (6,85).
   85 FORMAT ('1', 'IO ERROR ENCOUNTERED ON INPUT TAPE')
   STOP
   90003 WRITE (6,86).
   86 FORMAT ('1', 'ISTART IS LESS THAN OR EQUAL TO THE FIRST TIME
   X STEP AVAILABLE')
   STOP
   END
THIS PROGRAM CALCULATES THE REACTION RATES FOR ION-ATOM INTERCHANGE BETWEEN O PLUS AND N2.

THE POPULATION OF THE VIBRATIONALLY EXCITED LEVELS OF N2 AND THE VIBRATIONAL TEMPERATURE COME FROM THE OUTPUT TAPE OF PROGRAM BOLTDEV.

REAL * 4 NI, N2Z, NBOLT,KBOLT,KEFF,KVIBL,NLTOT,KPRIM
LOGICAL * 1 IMAGE(5151)
DIMENSION Z(89), N2Z(89), PHI(6,89), TV(89), EPSIL(6,89)
X ,NBOLT(6,89),KBOLT(89), KEFF( 89), RATIO(21), KVIBL(6)
X ,ILEVEL(6), TAUN (89), ALKBOL(21), ALKEFF(21), II(6), NLTOT(6,89)
X ,ARAY(21), ARAYI(21), GRID(8281)

DATA INPUT
READ (5,12,END=90000) DELZ,ZUPPER,DELT,TIMEX,MMMTIN,LINC,TINC
X ,LBOUND,TINC2
12 FORMAT (F4.0,F5.0,F6.0,F7.0,14,413)
WRITE (6,13) DELZ,ZUPPER,DELT,TIMEX,MMMTIN,LINC,TINC
X ,LBOUND, TINC2
13 FORMAT ('0',F4.0,F5.0,F6.0,F7.0,14,413)
READ (5,14,END=90000) DII,TI,NI,EPU,TOO
14 FORMAT (F6.4,F6.0,E13.7,F5.3,F5.0)
WRITE (6,15) DII,TI,NI,EPU,TOO
15 FORMAT ('0',F6.4,F6.0,E13.7,F5.3,F5.0)
READ (5,16,END=90000) (ILEVEL(N),KVIBL(N),N=1,6)
16 FORMAT (6(12,E9.1))
WRITE (6,17) (ILEVEL(N),KVIBL(N),N=1,6)
17 FORMAT('0',I12,E9.1)
LMAX = 1. + (ZUPPER - 120.)/DELZ
READ (5,18,END=90000) INCRTM,KPRIM,IPR
18 FORMAT(16,E9.1,16)
WRITE (6,19) INCRTM,KPRIM,IPR
19 FORMAT ('0',I16,1PE9.1,16)
READ (10,END=90001,ERR=90002) MIM,DELT1,LBOUND,DELZ
X ,DELZI,LINC,(Z(II),N2Z(II),TV(II),II(II),
X ,PHI(II,II), EPSIL(II,II), NBOLT(II,II),II=1,6,1),II=
X ,LBOUND,LMAX,LINC)
ITEST = MIM
JMAX = INCRTM - 1
DO 1000 M=1,10000,INCRTM
DO 1500 L=LBOUND,LMAX,LINC
SUM1 = 0.
SUM2 = 0.
DO 2000 J=1,6
NLTOT(J,L)= NBOLT(J,L) + EPSIL(J,L)
A = (KVIBL(J) - KPRIM)*NBOLT(J,L)
1000 CONTINUE
1500 CONTINUE
2000 CONTINUE
\[ B = KVIBL(J) \times EPSIL(J, L) \]
\[ SUM1 = SUM1 + A \]
\[ SUM2 = SUM2 + B \]
\[ TAUINV = SUM1 + KPRIM \times N2Z(L) \]
\[ TAUB(L) = 1./TAUINV \]
\[ TAUE(L) = 1./(TAUINV + SUM2) \]
\[ TAUN(L) = 1. / (1.3E-12 \times N2Z(L)) \]
\[ KBOLT(L) = KPRIM + SUM1/N2Z(L) \]
\[ KEFF(L) = KBOLT(L) + SUM2/N2Z(L) \]
\[ RATIOL(L) = KEFF(L) / KBOLT(L) \]
\[ ALTAUB(L) = ALOG10(TAUB(L)) \]
\[ ALTAUE(L) = ALOG10(TAUE(L)) \]
\[ ALTAUN(L) = ALOG10(TAUN(L)) \]
\[ ALKBOLT(L) = ALOG10(KBOLT(L)) \]
\[ ALKEFF(L) = ALOG10(KEFF(L)) \]

1500 CONTINUE

WRITE RESULTS TO TAPE.

C WRITE RESULTS TO TAPE.

WRITE (11) MMM, DELT1, LBOUND, DELZ, DELZ1
X LINCLZ(ILN), N2Z(ILN), TV(ILN), TAUB(ILN),
X TAUE(ILN), KBOLT(ILN), KEFF(ILN), RATIOK(ILN),
X (II(I), NBOLT(I), EPSIL(I), NLTOT(I, ILN),
X I = 1, 6, 1), ILN = LBOUND, LMAX, LINC

IF (MMM .NE. ITEST) GO TO 5000
ITEST = ITEST + IPR
WRITE (6, 20)
20 FORMAT ('1', 1X, 'MMM IS')
WRITE (6, 21) MMM
21 FORMAT ('+', 9X, I6)
WRITE (6, 50)
50 FORMAT ('0', 2X, 'ALT', 4X, 'TV', 4X, 'N(N2)', 9X, 'KBOLT', 9X,
WRITE (6, 51) (Z(ILN), TV(ILN), N2Z(ILN), KBOLT(ILN), KEFF(ILN),
X RATIOK(ILN), TAUN(ILN), TAUB(ILN), TAUE(ILN), ILN = LBOUND, LMAX, LINC)
51 FORMAT ('0', OPF5.0, OPF6.0, 1P7E14.6)

C PRINTER PLOT.

XR = 1000.
XL = 0.
YT = 11.
YB = 1.
NUMPRI = LMAX + 1
DO 3000 N = 1, 6
DO 3100 LL = LBOUND, LMAX, LINC
IF (LL .GE. 2) GO TO 3105
ARRAY(LL) = 1.
ARRAY1(II) = 1.
GO TO 3100
3105 ARRAY(LL) = ALOG10(NBOLT(N,LL))
ARRAY1(LL) = ALOG10(NLTOT(N,LL))
3100 CONTINUE
   WRITE (6,22)
22 FORMAT ('1',40X,'DENSITIES VERSUS ALTITUDE FOR')
   WRITE (6,23) N
23 FORMAT ('+',71X,12)
   CALL PLOT2(GRID,XR,XL,YT,YB)
   CALL PLOT3('+',Z,ARRAY,NUMPR1)
   CALL PLOT3('+',Z,ARRAY1,NUMPR1)
   CALL PLOT4(27,'LOG NUMBER DENSITY (CM**-3)')
   WRITE (6,24)
24 FORMAT ('0',59X,'ALTITUDE (KM.)')
3000 CONTINUE
   WRITE (6,25)
25 FORMAT ('1',40X,'REACTION RATES VERSUS ALTITUDE')
   YT = -9.
   YB = -14.
   CALL PLOT2(GRID,XR,XL,YT,YB)
   CALL PLOT3('+',Z,ALKBOL,NUMPR1)
   CALL PLOT3('+',Z,ALKEF,NUMPR1)
   CALL PLOT4(35,'LOG REACTION RATE (CM**3 SEC**-1)')
   WRITE (6,24)
24 FORMAT ('0',59X,'ALTITUDE (KM.)')
   YT = 1.5
   YB = 0.5
   WRITE (6,26)
26 FORMAT ('1',40X,'RATIO OF REACTION RATES')
   CALL PLOT2(GRID,XR,XL,YT,YB)
   CALL PLOT3('+',Z,RATIOK,NUMPR1)
   CALL PLOT4(20,'RATIO OF KEFF/KBOLT')
   WRITE (6,24)
24 FORMAT ('0',59X,'ALTITUDE (KM.)')
   YT = 5.
   YB = 0.
   WRITE (6,27)
27 FORMAT ('1',40X,'ELECTRON LOSS TIME CONSTANT')
   CALL PLOT2(GRID,XR,XL,YT,YB)
   CALL PLOT3('N',Z,ALTAUB,NUMPR1)
   CALL PLOT3('N',Z,ALTAUE,NUMPR1)
   CALL PLOT3('N',Z,ALTAUN,NUMPR1)
   CALL PLOT4(24,'LOG TIME CONSTANT (SEC.)')
5000 IF (INCRTM.EQ.1) GO TO 5500
   DO 5500 JJ=1,JMAX
5500 CONTINUE
   READ (10,END=90001,ERR=90002)
READ (10,END=90001,ERR=90002) MMM,DELT1,LBOUND,DELZ
X ,DELT1,LINC,(Z(ILN),N2Z(ILN),TV(ILN),(III(I),
X PHI(I,ILN),EPSIL(I,ILN),NBOLT(I,ILN),I=1,6,1),ILN=
X LBOUND,LMAX,LINC)
1000 CONTINUE
END FILE 11
90000 WRITE (6,33)
   END OF FILE ENCOUNTERED ON CARD READER
STOP
90001 WRITE (6,84)
   END OF FILE ENCOUNTERED ON INPUT TAPE
STOP
90002 WRITE (6,85)
   IO ERROR ENCOUNTERED ON INPUT TAPE
STOP
END