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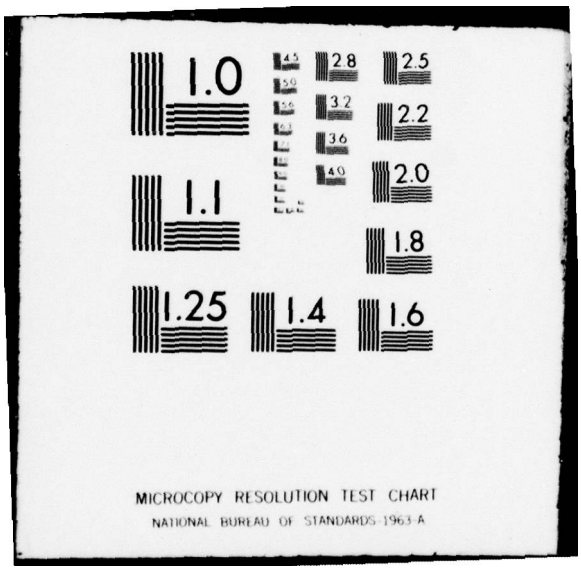
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Radial structure of a diffusion controlled, equilibrium oxygen discharge is modeled and analytically solved by using a Bessel substitution. A Maxwellian electron energy distribution is assumed. The initial model consists of electrons, O^-, O_2^-, and O_2^+ ions in background O_2 at 300°K. The reactions considered are dissociative attachment, associative detachment, and molecular ionization. The model is solved as a basic characteristic value problem for electron temperature. It is found that for a radius of 1.1cm at pressures of 0.2, 0.5, 1.0, and 5.0 torr, the equilibrium electron temperatures are 3.7, 2.2, 1.6, and 1.0 eV

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respectively; however, pR is not a scaling parameter. Results indicate that the O^- ion is the numerically dominant negative charge carrier and that it diffuses radially inward. The analytic technique is further applied to a four species, four reaction model which contains the O_2^- ion produced by charge transfer. An analytic solution of these models demonstrates a simple analytic scheme which may be used to solve other discharge models which contain more than four accompanying reactions.

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Preface

The research involved in thesis and the time spent on it has given me one of my most enjoyable and satisfying three months.

This has been due to the inspiration and delight that I have received in my association with my advisor, Dr. David A. Lee. I deeply appreciate the preponderance of patience, yet contagious enthusiasm which he always had with me and with my questions. Despite his harried schedule and numerous obligations, he always managed to produce an uninterrupted, scholarly atmosphere in which to discuss the problems that I encountered. The thesis presented herein is a product of the insight of this scholar and gentleman.

Thanks also are due to Professor Clarence R. Edstrom and Dr. John Jones, Jr., whose helpful suggestions have been utilized in many places throughout this thesis. And to Dr. Alan Garscadden whose timely suggestions kept the discharge model rolling, a debt of gratitude is owed.

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Frank D. Lewis

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Abstract

The radial structure of a diffusion controlled oxygen discharge at equilibrium is mathematically modeled, and is solved analytically by assuming a Maxwellian electron energy distribution and then using a Bessel substitution. A model consisting of electrons, O^-, and O_2^+ ions in background O_2 at 300°K along with the attendant reactions, dissociative attachment ($O_2 + e^- \rightarrow O^- + O$), its reverse ($O^- + O \rightarrow O_2 + e^-$), and ionization ($O_2 + e^- \rightarrow O_2^+ + 2e^-$), is solved analytically as a basic characteristic value problem for the electron temperature. It is found that for a tube radius of 1.1 cm and at pressures of 0.2, 0.5, 1.0, and 5.0 torr, the equilibrium electron temperatures are 3.7 eV, 2.2 eV, 1.6 eV, and 1.0 eV, respectively. The results also indicate that the O^- ion is the numerically dominant negative charge carrier and that it diffuses radially inward. The analytic technique is further applied to a four species, four reaction discharge model which contains the O_2^- ion and the charge transfer reaction ($O_2 + O^- \rightarrow O_2^- + O$). An analytic solution is found for this model. The pressure-radius product, pR, is not a scaling parameter. The solution of these models serves to prove the viability of a simple analytic scheme which may be used to solve other discharge models which contain more than four charged species and more than four accompanying reactions.

RADIAL STRUCTURE IN THE LOW PRESSURE EQUILIBRIUM OXYGEN DISCHARGE

I. Introduction

The universe is almost entirely composed of plasmas. Stars are gigantic plasmas. The relative void between the stars is filled with low density plasmas. Yet, man has evinced little interest in this ubiquitous phenomenon until a comparatively short time ago. Today, plasma research has blossomed into one of the dominant fields of scientific inquiry.

A plasma is an electrically conducting medium composed in general of charged particles, both positive and negative, whose properties depend on the collective behavior of the particles, as distinct from the individual. The present day theoretical effort to advance man's knowledge of the plasma state is founded on Lorentz's work in applying Boltzmann's particle kinetic theory to the behavior of electrons in metals and on wave particle kinetics. Since the 1950's, space exploration, electronic devices, gas discharge lasers, and the desire to achieve a controlled thermonuclear reactor have all stimulated interest in plasmas.

Some common examples of plasmas are auroras, lightning, welding arcs, and fluorescent lighting. The last is an example of an extended positive column discharge in an insulated glass tube. The discharge tube is an easy and convenient means of producing a plasma. An electrical potential is applied across a tube filled with gas and the electrons are driven to high kinetic energies. These energetic electrons in turn may cause ionization of the gas particles; thus a plasma is born.

Eventually, an equilibrium may be established within the discharge such that the production and loss of charged particles achieves a balance. Charged particles are lost and reborn through the reactions in which they participate. However, particles may also be lost as a result of radial migration to the walls of the discharge tube. In a plasma the different mobilities of electrons, positive ions, and negative ions induce electric fields which tend to retard the migration of the electrons and negative ions and which tend to accelerate the migration of the positive ions toward the tube wall. In this special case of radial migration, the combined diffusion of the electrons and ions forced by the space charge electric field is called "ambipolar diffusion" (Ref 18:417).

An example of a discharge system which has been observed experimentally off and on over the past fifty years and which is currently being investigated, is the oxygen discharge.

Oxygen Discharge Models

The oxygen discharge contains positive ions, negative ions, and electrons. It has been the subject of considerable research over the past fifty years because it is an atmospheric gas. Recently, it has been discovered that oxygen can be made to lase. This development has stimulated experimentation on the oxygen discharge system in an attempt to unravel the underlying plasma mechanisms, and thus to lay the groundwork for the design of an efficient lasing system.

The oxygen discharge system is made up of more than six different species and more than 170 processes (Ref 2:263-267). Because the system is relatively complex, it has withstood attempts at rigorous

mathematical analysis. However, some computer models have been recently developed to investigate it in detail (Ref 2).

The major species involved in the oxygen discharge may be qualitatively surmised by considering the electronegative character of oxygen and the production and loss mechanisms of the various species. At a gas temperature of around 300°K atomic oxygen, O, has an electron affinity of about 1.5 eV; and molecular oxygen, O_2, has an electron affinity of approximately 0.5 eV. Thus, it may be expected that both O^- and O_2^- ions will be formed in the presence of electrons.

Beginning with O_2, electrons, and an electric field, it is possible to produce O^- ions via dissociative attachment ($O_2 + e^- \rightarrow O^- + O$). The electron energy necessary for this reaction is the energy required to dissociate molecular oxygen minus the electron affinity of atomic oxygen or about 3.8 eV. Once O^- ions are produced, a continuous charge exchange process may begin ($O^- + O_2 \rightleftarrows O_2^- + O$) which produces O_2^- ions.

Positive ions are produced by ionization of both O_2 and O. Electrons with energies greater than about 12 eV will produce O_2^+ ions ($O_2 + e^- \rightarrow O_2^+ + 2e^-$), and electrons with energies greater than about 13.5 eV will produce O^+ ions ($O + e^- \rightarrow O^+ + 2e^-$). These ions may also be expected to participate in charge transfer reactions ($O_2^+ + O \rightleftarrows O^+ + O_2$). Dissociative ionization reactions require electrons with energies greater than 17 eV.

Loss of oxygen ions can occur by recombination. Radiative recombination events have very low cross sections (Ref 20:521). Therefore, the only important loss mechanisms are dissociative recombination and mutual neutralizations with dissociation. However, Thompson has shown that these recombination loss rates are much less than the

measured wall loss for diffusion dominated discharges in which the volume to surface ratio is much less than one (Ref 20:521).

Loss of oxygen ions can also occur by detachment. However, many of these reactions require ion temperatures greater than 1000°K; therefore, they are not significant loss mechanisms for discharges maintained at room temperature.

Of the species involved in the oxygen discharge, Thompson believes that the dominant ions are O^- and O_2^- negative ions, and O_2^+ positive ions (Ref 20:519). Using electrons, and the O^- and O_2^+ ions, Sabadil has modeled the oxygen discharge utilizing a numerical scheme (Ref 17). Recently, Lee has investigated an analytic solution to discharge systems (Ref 10). This thesis will attempt to verify that his mathematical technique and a limited account of the plasma chemistry gives reasonable results for the oxygen discharge.

The first simplified model analyzed will be a three species system containing electrons, and the O^- and O_2^+ ions. The reactions considered are dissociative attachment ($O_2 + e^- \rightarrow O^- + O$), its reverse ($O^- + O \rightarrow O_2 + e^-$), and ionization ($O_2 + e^- \rightarrow O_2^+ + 2e^-$).

Second, to this system will be added the charge transfer reaction ($O_2 + O^- \rightarrow O_2^- + O$), which is the primary means for producing the fourth species, O_2^- (Ref 20:522). The third and fourth models will include other reactions added to the four species discharge.

The discharge will be assumed to be contained within a long cylindrical tube whose dimensions are greater than the Debye length. The Debye length, λ_d, is the maximum distance in a plasma over which a large difference in the number of positive and negative charges can occur.

$$\lambda_d = 69\left(\frac{Te}{Ne}\right)^{\frac{1}{2}} \qquad (1.1)$$

Te is the electron temperature in °K, and Ne is the number density of electrons in m^{-3}. The Debye length, λ_d, is given in meters. For electron temperatures of 4×10^4 °K and electron densities of 10^{16} m^{-3}, the resulting Debye length is less than 0.05 cm. The radius of the discharge tube in this thesis is 1.1 cm and the length is considered to be greater than 1.0 m. Therefore, charge quasi-neutrality will be assumed to exist in all the discharge models examined.

Also, it will be assumed that electrons in the discharge may be described by a Maxwellian energy distribution. Actually, Dettmer provides evidence that the electron energy distribution is between a Maxwellian and a Druyvesteyn distribution (Ref 2:221). A Maxwellian distribution, successful in past discharge models, will be assumed here (Ref 11).

An analytic solution will be obtained for both the three and four species models.

Sequence of Development

In Chapter II, discharge equations developed from the first three moments of the Boltzmann equation for a three species model will be solved analytically as a basic characteristic value problem for electron temperature. It will be assumed that the electrons are Maxwellian, that the discharge tube has cylindrical symmetry, that there is no applied magnetic field, and that self-electric fields are negligible.

In order to obtain numerical results from the analytic solution of the three species model, it is necessary to know how the dissociative

attachment rate and ionization rate depend on the electron temperature. Chapter III and Chapter IV report the modeling of these reaction rates as functions of the electron temperature.

Chapter V presents the numerical results from the solution of the three species oxygen discharge model using the constants pertinent to oxygen and the results for the reaction rates obtained in Chapter III and Chapter IV.

In Chapter VI the oxygen discharge is modeled as a four species, four reaction system and solved analytically, again as a basic characteristic value problem. Numerical results are also presented.

In Chapter VII some other models are brought forth, and Chapter VIII and Chapter IX conclude the thesis with a discussion of the analytic technique used to evaluate the various models and with recommendations about other areas that could be appropriately pursued.

Notation

All equations are identified by sequence number according to the chapter or appendix in which they are located, e.g. (2.11) indicates equation eleven in Chapter II. Figures are identified in the same manner. Tables are identified simply by a Roman numeral in the order that they appear in the thesis.

II. An Equilibrium Model for the Three Species, Three Reaction Oxygen Discharges

A three species, three reaction model of the O_2 discharge at equilibrium can be developed from the first three moments of the Boltzmann equation. By specifying a cylindrical discharge geometry and by utilizing the assumptions relevant to the given discharge, a system of differential equations which models the discharge may be obtained. These differential equations will be called "general discharge equations."

The three species considered are electrons, negative atomic oxygen ions, and positive molecular oxygen ions. They are represented as e^-, O^-, and O_2^+. Also involved are the background neutral oxygen molecules O_2, and the neutral oxygen atoms O.

The three reactions used in the model are as follows:

Name	Reaction	Rate $(\frac{1}{sec})$	
Dissociative Attachment	$O_2 + e^- \rightarrow O^- + O$	$\alpha(T_e)$	(2.1)
Atomic Detachment	$O^- + O \rightarrow O_2 + e^-$	γ	(2.2)
Molecular Ionization	$O_2 + e^- \rightarrow O_2^+ + 2e^-$	$\beta(T_e)$	(2.3)

Both the dissociative attachment rate α and the ionization rate β are modeled as functions of the Maxwellian electron temperature T_e. Also, α and β are linear functions of the background gas number density No_2. The detachment rate γ will be assumed a function of the atomic oxygen number density only.

The discharge is assumed to occur in a long cylindrical tube when an external electric field is applied along the axis of the tube. The cylindrical coordinates are (r, ϕ, z) with z along the tube axis.

The electric field in the tube will be described as

$$\underline{E} = [E_r(r), 0, E_o] \tag{2.4}$$

The average velocities of the three species are $\underline{q}_e$, $\underline{q}_-$, and $\underline{q}_+$. The subscripts represent e^-, O^-, and O_2^+, respectively. These average velocities will be modeled with the following components:

$$\underline{q}_e = [v_e(r),o,u_e]; \ \underline{q}_- = [v_-(r),o,u_-]; \ \underline{q}_+ = [v_+(r),o,u_+] \tag{2.5}$$

The axial components of the average velocities for each species are u_e, u_-, and u_+. They are the drift velocities down the tube and will be assumed to be constant or at least that their derivatives with respect to the radial distance, r, will be negligibly small. This is a reasonable assumption for a constant potential applied across the ends of a long, narrow discharge tube.

With these preliminaries completed, it is now possible to examine the three species, three reaction discharge in detail. First, the "general discharge equations" will be reduced to "specific discharge equations." Second, these "specific discharge equations" will be partially solved to obtain the "essential discharge equations." Third, a magic substitution will be made to change these essential differential equations into a tractable set of algebraic equations. And finally, this set of algebraic equations will be solved. Their solution will constitute an analytic solution to the three species, three reaction oxygen discharge.

Reduction of the General Discharge Equations

In view of the specific setup outlined above, the general discharge equations consist of the particle conservation equations, which are:

$$v_e n_e' + n_e v_e' + \frac{n_e v_e}{r} = (\beta - \alpha) n_e + \gamma n_- \tag{2.6}$$

$$v_- n_-' + n_- v_-' + \frac{n_- v_-}{r} = \alpha n_e - \gamma n_- \tag{2.7}$$

$$v_+ n_+' + n_+ v_+' + \frac{n_+ v_+}{r} = \beta n_e \tag{2.8}$$

The prime indicates differentiation with respect to the radial distance r. The radial momentum conservation equations are

$$v_e v_e' = \frac{-1}{n_e m_e}(T_e n_e)' - \frac{q_o}{m_e} E_r - \nu_e v_e \tag{2.9}$$

$$v_- v_-' = \frac{-1}{n_- m_-}(T_- n_-)' - \frac{q_o}{m_-} E_r - \nu_- v_- \tag{2.10}$$

$$v_+ v_+' = \frac{-1}{n_+ m_+}(T_+ n_+)' + \frac{q_o}{m_+} E_r - \nu_+ v_+ \tag{2.11}$$

The axial momentum conservation equations are

$$v_e u_e' = \frac{-q_o}{n_e} E_o - \nu_e (u_e - u_o) \tag{2.12}$$

$$v_- u_-' = \frac{-q_o}{m_-} E_o - \nu_- (u_- - u_o) \tag{2.13}$$

$$v_+ u_+' = \frac{q_o}{m_+} E_o - \nu_+ (u_+ - u_o) \tag{2.14}$$

The energy conservation equations are

$$v_e T_e' = -\frac{2}{3} T_e (v_e' + \frac{v_e}{r}) + \frac{2}{3} m_e \nu_e (v_e^2 + u_e^2) - \frac{2}{3} \nu_{eo} T_e \tag{2.15}$$

$$v_- T_-' = -\frac{2}{3} T_- (v_-' + \frac{v_-}{r}) + \frac{2}{3} m_- \nu_- (v_-^2 + u_-^2) - \frac{2}{3} \nu_{-o} (T_- - T_o) \tag{2.16}$$

$$v_+T_+' = -\frac{2}{3}T_+(v_+' + \frac{v_+}{r}) + \frac{2}{3}m_+\nu_+(v_+^2 + u_+^2) - \frac{2}{3}\nu_{+o}(T_+ - T_o) \quad (2.17)$$

And Poisson's equation is

$$E_r' + \frac{E_r}{r} = \frac{q_o}{\varepsilon_o}(n_+ - n_e - n_-) \quad (2.18)$$

A detailed derivation of results which lead directly to these equations is contained in Appendix A and Appendix B.

The primes indicate differentiation with respect to the radial distance, r. The quantities n_e, n_-, and n_+ are the number densities of the indicated species. T_e, the Maxwellian electron temperature, is in units of ergs and therefore is normalized by the Boltzmann constant. T_- and T_+ are the energy temperatures of the indicated species. m_e, m_-, and m_+ represent the masses of the species. q_o is the unit electrostatic charge and ε_o is the permittivity constant. ν_e, ν_-, and ν_+ are the collision frequencies of the indicated species with the neutral background gas, O_2, multiplied by the fractional momentum loss each species suffers per collision. Likewise, ν_{eo}, ν_{-o}, and ν_{+o} are the collision frequencies of the species with O_2's multiplied by the fractional energy loss each species suffers on impact.

Now let

$$j_e = n_e v_e; \quad j_- = n_- v_-; \quad j_+ = n_+ v_+ \quad (2.19)$$

Where j_e, j_-, and j_+ are the radial current densities for each species. The particle conservation equations become

$$j_e' + {}^{j_e}/_r = (\beta - \alpha)n_e + \gamma n_- \quad (2.20)$$

$$j_-' + {}^{j_-}/_r = \alpha n_e - \gamma n_- \quad (2.21)$$

$$j_+' + {}^{j_+}/_r = \beta n_e \tag{2.22}$$

The radial momentum equations (2.9), (2.10), and (2.11) may be simplified by assuming that

$$v_e v_e' << \frac{T_e n_e'}{n_e m_e}, \frac{q_o}{m_e} E_r, v_e \nu_e \tag{2.23}$$

$$v_- v_-' << \frac{T_- n_-'}{n_- m_-}, \frac{q_o}{m_-} E_r, v_- \nu_- \tag{2.24}$$

$$v_+ v_+' << \frac{T_+ n_+'}{n_+ m_+}, \frac{q_o}{m_+} E_r, v_+ \nu_+ \tag{2.25}$$

These are reasonable assumptions for a discharge tube with a 1 cm radius operated at pressures of 5 torr or less. The electron inequalities may be demonstrated using representative values for the parameters involved. For electrons with a 1 eV temperature, T_e is on the order of 10^{-12} erg. Typical radial electron velocities are about 10^5 cm/sec. v_e' for a 1 cm radius tube may be approximated as 10^5 sec^{-1} since $v_e(o)$ must be zero to preclude non-singular fields. This is probably a generous estimate. It is assumed that electrons will recombine at the tube wall. Then n_e'/n_e may be approximated by unity. ν_e may be obtained from mobilities and is approximately 10^9 sec^{-1}. q_o is 1.6×10^{-12} erg/volt. The mass of the electron is about 10^{-27} g. It is assumed that the radial electric field, E_r, is much greater than 10^{-4} volt/cm. Then $v_e v_e'$ is much less than the quantities on the right of (2.23) and may be neglected when compared to them. A similar demonstration may be made for the ions.

It is assumed that at equilibrium T_e, T_-, and T_+ are constant. Utilizing (2.19) and these assumptions, the radial momentum equations become

$$j_e = \frac{-T_e}{m_e \nu_e} n_e' - \frac{q_o}{m_e \nu_e} n_e E_r \tag{2.26}$$

$$j_- = \frac{-T_-}{m_- \nu_-} n_-' - \frac{q_o}{m_- \nu_-} n_- E_r \tag{2.27}$$

$$j_+ = \frac{-T_+}{m_+ \nu_+} n_+' + \frac{q_o}{m_+ \nu_+} n_+ E_r \tag{2.28}$$

It has already been assumed that u_e', u_-', and u_+' are negligibly small. Assume that the axial component of velocity for the neutrals, u_o, may be neglected when compared to the axial components of velocity for the species, because only the charged particles are accelerated by the applied electric field. This is reasonable for a discharge in which the fractional ionization is extremely small or several orders of magnitude less than unity. This same assumption could be made if the neutral particles were pumped through the discharge tube with a velocity equal and opposite to the net velocity imparted to them by the charged particles. Then the axial momentum equations may be written

$$u_e = \frac{-q_o}{m_e \nu_e} E_o \tag{2.29}$$

$$u_- = \frac{-q_o}{m_- \nu_-} E_o \tag{2.30}$$

$$u_+ = \frac{q_o}{m_+ \nu_+} E_o \tag{2.31}$$

The energy equations may be simplified by comparing terms as was done with the radial momentum equations. Assume that $u_e >> v_e$, which is assuming that the drift speed of the electrons along the tube is much

greater than the diffusion speed of the electrons along the radii. Also, assume that $\nu_e \simeq \nu_{eo}$ whereas $\nu_- << \nu_{-o}$ and $\nu_+ << \nu_{+o}$. This is reasonable since O^- and O_2^- ions are about the same size as the background O_2; therefore, O^- and O_2^+ will have a large energy coupling with the O_2. The electrons are very weakly coupled to the O_2. Remembering that T_e, T_-, and T_+ are constant at equilibrium, the energy conservation equations may be written as

$$T_e = \frac{m_e \nu_e}{\nu_{eo}} u_e^2 \tag{2.32}$$

$$T_- = T_o \tag{2.33}$$

$$T_+ = T_o \tag{2.34}$$

Lee obtains this result by a non-dimensionalization of the same general energy equations (Ref 9:1-7).

The original "general moment equations" have been reduced to "specific moment equations" for the three species, three reaction oxygen discharge. These "specific moment equations" are the particle conservation equations.

$$j_e' + {}^{j_e}/_r = (\beta - \alpha) n_e + \gamma n_- \tag{2.20}$$

$$j_-' + {}^{j_-}/_r = \alpha n_e - \gamma n_- \tag{2.21}$$

$$j_+' + {}^{j_r}/_r = \beta n_e \tag{2.22}$$

the radial momentum conservation equations

$$j_e = \frac{-T_e}{m_e \nu_e} n_e' - \frac{q_o}{m_e \nu_e} n_e E_r \tag{2.26}$$

$$j_- = \frac{-T_-}{m_- \nu_-} n_-' - \frac{q_o}{m_- \nu_-} n_- E_r \tag{2.27}$$

$$j_+ = \frac{-T_+}{m_+ \nu_+} n_+' + \frac{q_o}{m_+ \nu_+} n_+ E_r \tag{2.28}$$

the axial momentum conservation equations

$$u_e = \frac{-q_o}{m_e \nu_e} E_o \tag{2.29}$$

$$u_- = \frac{-q_o}{m_- \nu_-} E_o \tag{2.30}$$

$$u_+ = \frac{q_o}{m_+ \nu_+} E_o \tag{2.31}$$

the energy equations

$$T_e = \frac{m_e \nu_e}{\nu_{eo}} u_e^2 \tag{2.32}$$

$$T_- = T_+ = T_o \tag{2.35}$$

and Poisson's equation

$$E_r' + \frac{E_r}{r} = \frac{q_o}{\varepsilon_o} (n_+ - n_e - n_-) \tag{2.18}$$

This system of equations is used by Lee at the outset of his solution for the identical discharge (Ref 10:1).

The Essential Discharge Equations

The methodology here will closely follow Lee's treatment of the three moment, three reaction gas discharge (Ref 10:1-8).

For the specific discharge system above, it is assumed that the background gas temperature, T_o, is known. The ionic species temperature will be represented as T_o.

The specific discharge system of equations is (2.20), (2.21), (2.22), (2.26), (2.27), (2.28), (2.30), (2.31), (2.32), and (2.18). Thus there are eleven equations in the eleven unknowns j_e, j_-, j_+, u_e, u_-, u_+, n_e, n_-, n_+, E_r, and E_o.

Boundary Conditions. The boundary conditions which will close the system must be specified. In order to retain system symmetry and to preclude non-singular fields, it is necessary that at r = 0 the following be true:

$$n_e'(o) = n_-'(o) = n_+'(o) = 0 \tag{2.36}$$

$$j_e(o) = j_-(o) = j_+(o) = 0 \tag{2.37}$$

$$E_r(o) = 0 \tag{2.38}$$

Now at r = R, the wall of the tube, it is assumed that recombination of the charged particles occurs. Also the net current should be zero. Thus,

$$j_+(R) - j_e(R) - j_-(R) = 0 \tag{2.39}$$

$$n_+(R) = n_e(R) = n_-(R) = 0 \tag{2.40}$$

This system of eleven specific discharge equations (four ordinary linear differential equations, three ordinary non-linear differential equations, three linear algebraic equations, and a single quadratic equation), eleven unknowns, and eleven boundary conditions constitute the model

for the three species, three reaction oxygen discharge. Only seven boundary conditions are required for a solution. The four extra boundary conditions came from the original differential equations (2.6) through (2.18).

Beginning the Solution. It is reasonable to assume quasi-neutrality in the positive column which excludes the plasma sheath near the wall of the tube (Ref 17:234). Thus,

$$n_+ = n_- + n_e \tag{2.41}$$

Only the following equations are pertinent for beginning a quasi-neutral solution:

$$j_e' + {}^{j_e}/_r = (\beta - \alpha)n_e + \gamma n_- \tag{2.20}$$

$$j_-' + {}^{j_-}/_r = \alpha n_e - \gamma n_- \tag{2.21}$$

$$j_+' + {}^{j_+}/_r = \beta n_e \tag{2.22}$$

$$j_e = \frac{-T_e}{m_e \nu_e} n_e' - \frac{q_o}{m_e \nu_e} n_e E_r \tag{2.26}$$

$$j_- = \frac{-T_o}{m_- \nu_-} n_-' - \frac{q_o}{m_- \nu_-} n_- E_r \tag{2.27}$$

$$j_+ = \frac{-T_o}{m_+ \nu_+} n_+' + \frac{q_o}{m_+ \nu_+} n_+ E_r \tag{2.28}$$

Now let

$$j \equiv j_+ - j_e - j_- \tag{2.42}$$

Then (2.20), (2.21), and (2.22) become

$$j' + j/_r = 0 \tag{2.43}$$

Using the boundary condition $j(R) = 0$ and solving yields

$$j_+ = j_- + j_e \tag{2.44}$$

This is the ambipolarity result. Also,

$$j_+' = j_-' + j_e' \tag{2.45}$$

This eliminates equation (2.22) from the system. j_+ and n_+ in equation (2.28) may be eliminated by using the results (2.44) and (2.41):

$$j_e + j_- = \frac{-T_o(n_e + n_-)'}{m_+\nu_+} + \frac{q_o E_r(n_e + n_-)}{m_+\nu_+} \tag{2.46}$$

E_r must be eliminated. Equations (2.26) and (2.27) can be written

$$n_e E_r = \frac{-T_e n_e'}{q_o} - \frac{m_e \nu_e}{q_o} j_e \tag{2.47}$$

$$n_- E_r = \frac{-T_o n_-'}{q_o} - \frac{m_- \nu_-}{q_o} j_- \tag{2.48}$$

Now,

$$n_- n_e E_r = n_e n_- E_r \tag{2.49}$$

Therefore,

$$T_e n_- n_e' + m_e \nu_e n_- j_e = T_o n_e n_-' + m_- \nu_- n_e j_- \tag{2.50}$$

If equations (2.26) and (2.27) are substituted into equation (2.46) and the result manipulated slightly, the following equation results:

$$j_e(m_+\nu_+ + m_e\nu_e) + j_-(m_+\nu_+ + m_-\nu_-) = -(T_e + T_o)n_e' - 2T_o n_-' \quad (2.51)$$

Then the entire model is reduced to the four "essential discharge equations":

$$j_e' + {}^{j_e}/_{r} = (\beta - \alpha)n_e + \gamma n_- \quad (2.20)$$

$$n_-' + {}^{j_-}/_{r} = \alpha n_e - \gamma n_- \quad (2.21)$$

$$j_e(m_+\nu_+ + m_e\nu_e) + j_-(m_+\nu_+ + m_-\nu_-) = -(T_e + T_o)n_e' - 2T_o n_-' \quad (2.51)$$

$$T_e n_- n_e' + m_e\nu_e n_- j_e = T_o n_e n_-' + m_-\nu_- n_e j_- \quad (2.50)$$

The boundary conditions require $n_e(o)$ and $n_-(o)$ to be bounded and

$$n_e'(o) = n_-'(o) = 0 \quad (2.52)$$

$$n_e(R) = n_-(R) = 0 \quad (2.53)$$

This is the basic characteristic value problem for T_e. It must be remembered that the production rates α and β depend on T_e.

The Magic Substitution

The essential discharge equations consist of three linear first order differential equations and one non-linear first order differential equation. Even though the system is a basic characteristic value problem for T_e, finding an analytic solution to it appears to be

insidiously intractable. Using equations identical to (2.20), (2.21), (2.26), (2.27), and (2.28), Sabadil does find a numerical solution to the discharge (Ref 17:236).

However, Lee (Ref 10:5) suggests the magic substitutions

$$j_\lambda = J_\lambda J_1(\sigma_1 r) \tag{2.54}$$

$$n_\lambda = N_\lambda J_0(\sigma_1 r) \tag{2.55}$$

The subscript λ indicates all species. J_λ and N_λ are constant current densities and number densities, respectively. J_1 is the first order Bessel function and J_0 is the zeroth order Bessel function. The argument of these Bessel functions is defined as

$$\sigma_1 = \frac{\zeta_1}{R} \tag{2.56}$$

where R is the radius of the discharge tube. Also,

$$J_0(\zeta_1) = 0 \tag{2.57}$$

where ζ_1 is the first zero of J_0. This is similar to the Schottky method for analyzing a much simpler positive column (Ref 21:238-243).

It can be shown that

$$j_\lambda' + {}^{j_\lambda}/_r = \sigma_1 J_\lambda J_0(\sigma_1 r) \tag{2.58}$$

$$n_\lambda' = -\sigma_1 N_\lambda J_1(\sigma_1 r) \tag{2.59}$$

The boundary conditions at r = 0 and r = R are still met.

Substituting (2.54), (2.55), (2.58), and (2.59) into the essential discharge equations, and assuming that $T_e \gg T_0$ and $m_+\nu_+ \gg m_e\nu_e$ results in the system

$$(\beta - \alpha)N_e + \gamma N_- - \sigma_1 J_e + 0 = 0 \qquad (2.60)$$

$$\alpha N_e - \gamma N_- + 0 - \sigma_1 J_- = 0 \qquad (2.61)$$

$$\sigma_1 T_e N_e + 2\sigma_1 T_o N_- - m_+\nu_+ J_e - (m_+\nu_+ + m_-\nu_-)J_- = 0 \qquad (2.62)$$

$$-\sigma_1 T_e N_- N_e + \sigma_1 T_o N_e N_- + m_e\nu_e N_- J_e - m_-\nu_- N_e J_- = 0 \qquad (2.63)$$

Thus, Lee's magic substitution has changed the intractable set of linear and non-linear differential equations into a tractable set of three linear and one non-linear algebraic equations.

Solution

The solution to the three species, three reaction model of the oxygen discharge has been reduced to solving a system of four algebraic equations. The system may be written

$$\begin{pmatrix} \gamma & -\sigma_1 & 0 \\ -\gamma & 0 & -\sigma_1 \\ 2T_o\sigma_1 & -m_+\nu_+ & -(m_+\nu_+ + m_-\nu_-) \end{pmatrix} \begin{pmatrix} \frac{N_-}{N_e} \\ \frac{J_e}{N_e} \\ \frac{J_-}{N_e} \end{pmatrix} = \begin{pmatrix} \alpha - \beta \\ -\alpha \\ -\sigma_1 T_e \end{pmatrix} \qquad (2.64)$$

$$\sigma_1(-T_e + T_o)\frac{N_-}{N_e} + m_e\nu_e \left|\frac{N_-}{N_e}\right|\left|\frac{J_e}{N_e}\right| - m_-\nu_- \left|\frac{N_-}{N_e}\right|\left|\frac{J_-}{N_e}\right| = 0 \qquad (2.65)$$

The linear system (2.64) can be solved for $\frac{N_-}{N_e}$, $\frac{J_e}{N_e}$, and $\frac{J_-}{N_e}$. Thus,

$$\frac{N_-}{N_e} = \frac{-\sigma_1^3 T_e + \sigma_1\alpha m_-\nu_- + \sigma_1\beta m_+\nu_+}{2\sigma_1^3 T_o + \alpha\sigma_1 m_-\nu_-} \qquad (2.66)$$

$$\frac{J_e}{N_e} = \frac{-2\sigma_i^2 T_o(\alpha + \beta) + \beta\gamma(m_+\nu_+ + m_-\nu_-) - \sigma_i^2 T_e\gamma}{2\sigma_i^3 T_o + \gamma\sigma_i m_-\nu_-} \tag{2.67}$$

$$\frac{J_-}{N_e} = \frac{2\sigma_i^2 T_o\alpha - \beta\gamma m_+\nu_+ + \sigma_i^2 T_e\gamma}{2\sigma_i^3 T_o + \gamma\sigma_i m_-\nu_-} \tag{2.68}$$

A further simplification is possible. By algebraically carrying out the division in equation (2.66), it is seen that

$$\frac{N_-}{N_e} = \frac{\alpha}{\gamma} + \frac{\sigma_i/\gamma\left[-\sigma_i^2 T_e\gamma + \beta\gamma m_+\nu_+ - 2\sigma_i^2 T_o\alpha\right]}{2\sigma_i^3 T_o + \gamma\sigma_i m_-\nu_-} \tag{2.69}$$

Then,

$$\frac{N_-}{N_e} = \frac{\alpha}{\gamma} + \frac{\sigma_i}{\gamma}\left[\frac{J_-}{N_e}\right] \tag{2.70}$$

By rearranging equation (2.67), it may be shown that

$$\frac{J_e}{N_e} = \frac{\beta}{\sigma_i} - \left[\frac{J_-}{N_e}\right] \tag{2.71}$$

Results (2.70) and (2.71) may be substituted into equation (2.65):

$$\sigma_i m_e\nu_e\left[\frac{J_-}{N_e}\right]^2 + \left[\sigma_i^2(T_e - T_o) - m_e\nu_e(\alpha + \beta) - \gamma m_-\nu_-\right]$$

$$+\left[\left[\frac{\alpha\beta}{\sigma_i}\right]m_e\nu_e - \sigma_i\alpha(T_e - T_o)\right] = 0 \tag{2.72}$$

This is the characteristic value equation for T_e . When it is solved, the three species, three reaction oxygen discharge model that has

been postulated will be determined. Equation (2.72) is solved by iterating it with T_e to find the zeroes. Once the equilibrium T_e has been found, it is possible to determine the remaining unknowns in the model.

Using the equilibrium value of T_e and applying equation (2.32), the axial electron drift speed is

$$u_e = \left(\frac{T_e \nu_{eo}}{m_e \nu_e} \right)^{\frac{1}{2}} \tag{2.73}$$

Because the fractional energy loss is the sum of the elastic as well as the inelastic processes, determining the value of ν_{eo} for use in this equation is not trivial.

Equation (2.29) yields the equilibrium axial electric field:

$$E_o = \frac{-m_e \nu_e u_e}{q_o} \tag{2.74}$$

Then u_- and u_+ are determined by

$$u_- = - \frac{q_o E_o}{m_- \nu_-} \tag{2.30}$$

$$u_+ = \frac{q_o E_o}{m_+ \nu_+} \tag{2.31}$$

Experimental and theoretical information on the equilibrium electric field versus the current necessary to run the oxygen discharge at various pR values is available. Dettmer, in his thesis, has calculated such curves for the oxygen discharge (Ref 2:38). Of course, the model of the discharge herein, with the resultant equation (2.74),

predicts an electric field independent of current. Since it is possible to postulate a value for the discharge current, I, at the equilibrium E_o, it is possible to compute values for N_e, N_-, and N_+ (Ref 11):

$$I = 2\pi q_o \int_o^R (n_+ u_+ - n_- u_- - n_e u_e) r \, dr \tag{2.75}$$

Charge quasi-neutrality has previously been assumed. Utilizing equations (2.54) and (2.55), equation (2.75) becomes

$$I = 2\pi q_o N_e \left[(u_+ - u_e) + \frac{N_-}{N_e}(u_+ - u_-)\right] \int_o^R r J_o(\sigma_1 r) dr \tag{2.76}$$

Then,

$$N_e = \frac{I\zeta_1}{2\pi q_o N_e \left[(u_+ - u_e) + \frac{N_-}{N_e}(u_+ - u_-)\right] R^2 J_1(\zeta_1)} \tag{2.77}$$

Equation (2.77) determines N_e and thus n_e. As a result N_- and n_- are determined. Then n_+ is determined by charge neutrality.

The ratios $\frac{J_e}{N_e}$ and $\frac{J_-}{N_e}$ have already been determined. Given N_e, the radial density constants J_e and J_- are determined. Therefore, j_e and j_- are determined, and j_+ results from applying the ambipolarity equation (2.44).

Finally, the radial electric field E_r is obtained from equation (2.47) or (2.48). Using the magic substitutions as well as (2.59) it may be seen that

$$E_r = \left[\frac{\sigma_1 T_e}{q_o} - \frac{m_e \nu_e}{q_o} \cdot \frac{J_e}{N_e}\right] \frac{J_1(\sigma_1 r)}{J_o(\sigma_1 r)} \tag{2.78}$$

This completes the determination of the three species, three reaction oxygen discharge model.

The Model Inconsistency

The three species, three reaction discharge model which has been developed is actually inconsistent. But this is the normal inconsistency associated with the Schottky ambipolar diffusion model with Bessel profiles (Ref 11). Using equation (2.19) and the magic substitutions (2.54) and (2.55), it is easily shown that the radial velocities of each species are

$$v_\lambda = \frac{J_\lambda}{N_\lambda} \cdot \frac{J_1(\sigma_1 r)}{J_0(\sigma_1 r)} \tag{2.79}$$

Equations (2.78) and (2.79) make it clear that E_r and v_λ blow up at the tube wall, r = R, where $\sigma_1 r = \zeta_1$, the first zero of J_0 (see Figure 2-1).

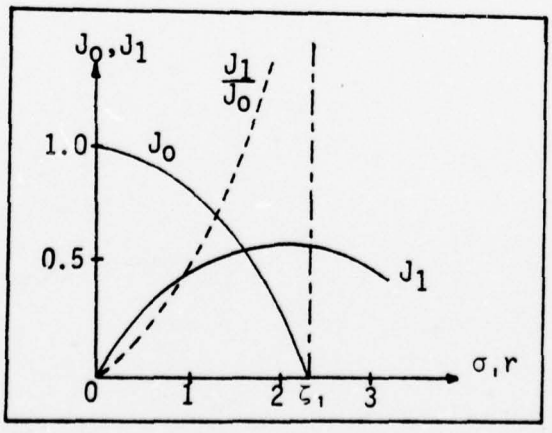

Figure 2-1. Inconsistencies Due to Bessel Profiles

Mitchner and Kruger have shown that the ambipolar diffusion model begins to fail at a distance from the tube wall which usually is negligibly small (Ref 13:150-154). Lee approximates the distance as 10^{-4}xR (Ref 9:12). The region near the tube wall is the plasma sheath; and modeling it into the discharge would require a discharge model much more sophisticated than the simple one postulated herein. It is assumed that the distance from the tube wall at which the present model begins to fail is very small. Therefore, while realizing that an inconsistency does in fact exist in this model, its presence will be ignored.

Summary

It has been demonstrated that an analytic solution to a simple three species, three reaction model of the oxygen discharge does theoretically exist. The agility of the model is a result of Lee's magic substitution (Ref 10:5). It remains to be demonstrated that this theoretical solution has physical significance.

Earlier it was pointed out that the dissociative attachment rate α and the total ionization rate β were being modeled as functions of the Maxwellian electron temperature T_e. In order to solve the characteristic value equation (2.72) for T_e, it is necessary to know the functional dependence of α and β on T_e.

III. The Dissociative Attachment Rate

In order to utilize the model solution obtained in Chapter II, it is necessary to know how the dissociative attachment rate α depends on the Maxwellian electron temperature T_e. The dissociative attachment reaction makes it obvious that α is highly dependent on T_e:

$$O_2 + e^- \rightarrow O^- + O \tag{2.1}$$

α as a function of electron energy, E, may be obtained in a manner similar to the method employed by von Engel (Ref 21:292-293). A result found in most plasma textbooks and demonstrated by Nielsen (Ref 15:26, 34) is that the probability for a dissociative attachment event, P_d, occurring is

$$P_d = \sigma(E)\left[\frac{2E}{m_e}\right]^{\frac{1}{2}} \tag{3.1}$$

Here $\sigma(E)$ is the total collision cross section for dissociative attachment as a function of the electron kinetic energy E. Assume that the electron energy distribution is the Maxwellian

$$N(E)dE = n_e \frac{2}{\sqrt{\pi}} (T_e)^{-3/2} E^{\frac{1}{2}} e^{-E/T_e}\, dE \tag{3.2}$$

Then the dissociative attachment rate is

$$\alpha(T_e) = \int_{E_c}^{\infty} N_{O_2} P_d(E) N(E) dE \tag{3.3}$$

E_c is the threshold energy for the dissociative attachment process. N_{O_2} is the background O_2 number density. Substituting (3.1) and

(3.2), one sees that the rate α satisfies

$$\frac{\alpha(T_e)}{N_{O_2}} = \frac{2}{\sqrt{\pi}} T_e^{-3/2} \int_{E_c}^{\infty} \sigma(E) \left(\frac{2E}{m_e}\right)^{\frac{1}{2}} E^{\frac{1}{2}} e^{-E/T_e} dE \qquad (3.4)$$

First, the collision cross section dependence on the electron energy will be determined. Second, using the determined $\sigma(E)$, the integral of equation (3.4) will be evaluated.

Cross Section Dependence on Electron Energy

Cross section $\sigma_d(E)$ versus electron energy E data for dissociative attachment in oxygen is available in the JILA Report (Ref 7:98-101). These data were analyzed with a Hewlett-Packard HP-67 calculator. The data, when graphed, assume a bell-shaped profile (See Figure 3-1). The data which were used were for O_2 at a temperature of about 350°K. Data for O_2 at temperatures as high as 1030°K were shifted only slightly toward lower energy values.

Following von Engel (Ref 21:292-293), $\sigma_d(E)$ would be approximated as the best linear fit to the leading edge of the data curve. In most cases this is quite satisfactory, because it is only the meagre supply of electrons in the tail of the Maxwellian electron distribution which make it past the threshold energy E_c, i.e., usually the tail of the electron distribution goes to zero under the leading edge of the bell-shaped $\sigma_d(E)$ curve.

However, in this model it was not clear that such a linear approximation would be adequate; therefore, an analytic curve, $\sigma_d(E)$, was determined which had the same bell-shaped profile as the entire data set. Even if this approach were needless fine tuning for a model based on a Maxwellian distribution, it would still serve to limit the number

of assumptions made. The analytic curve was determined in two steps.

First, using the HP-67 "Curve Fitting" program (Ref 6:03-01, L03-01) and adjusting the collision data to the program coordinate system, a reasonable power curve fit to the forward edge of the data was found to be

$$\sigma_d(E) = 2.35 \times 10^{-19}(E-3.8)^2 \tag{3.5}$$

Where 3.8 eV is assumed to be the threshold electron energy for dissociative attachment, E_c.

Second, in order to bend the curve over, $\sigma_d(E)$ was assumed to be of the form

$$\sigma_d(E) = a(E-3.8)^b e^{-c(E-3.8)^2} \tag{3.6}$$

Where the constants, a and c, are assumed to be in units of $cm^2 \cdot eV^{-b}$ and eV^{-2}, respectively. This equation was programmed into the HP-67 and iterated, varying the parameters a, b, and c. The best curve fit to the data was determined by eye. It was found to be

$$\sigma_d(E) = (2.75 \times 10^{-19})(E-3.8)^3 e^{-0.19(E-3.8)^2} \tag{3.7}$$

The data and analytic curve (3.7) are shown in Figure 3-1.

Determination of $\alpha(T_e)/N_{O_2}$

The dissociative attachment rate $\alpha(T_e)/N_{O_2}$ in units of $cm^3 \cdot sec^{-1}$ may be expressed, with the aid of equations (3.4) and (3.7), as

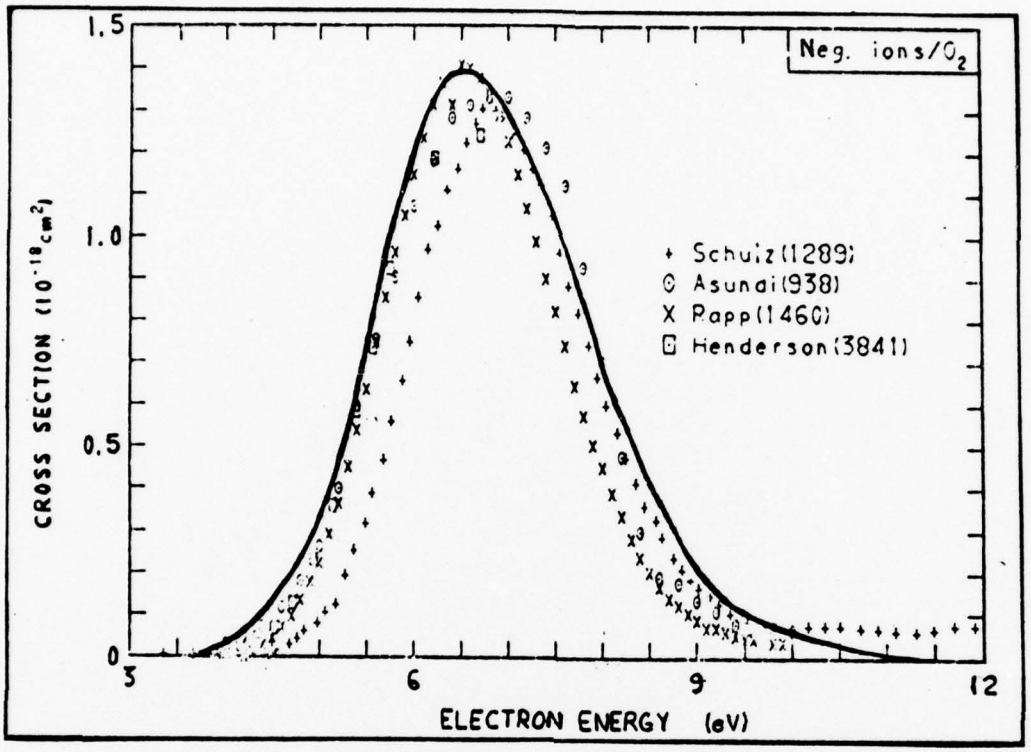

Figure 3-1. Data and Analytic Curve for Dissociative Attachment Cross Section vs. Electron Energy in Oxygen (Ref 7:98)

$$\frac{\alpha(T_e)}{No_2} = \frac{2}{\sqrt{\pi}} T_e^{-3/2} \int_{E_c}^{\infty} (2.75 - 10^{-19})(E-3.8)^3 e^{-0.19(E-3.8)^2} \left(\frac{2E^*}{m_e}\right)^{\frac{1}{2}} E^{\frac{1}{2}} e^{-E/T_e} dE \tag{3.8}$$

In order to express all energies in eV's, it was necessary to convert E in ergs in the velocity term to eV's:

$$(E^*)^{\frac{1}{2}}(ergs)^{\frac{1}{2}} = E^{\frac{1}{2}}(eV)^{\frac{1}{2}} \times (1.2657)(10^{-6})\left(\frac{erg}{eV}\right)^{\frac{1}{2}} \tag{3.9}$$

Combining all constants and using (3.9), equation (3.8) becomes

$$\frac{\alpha(T_e)}{No_2} = \frac{(1.840411 \times 10^{-11})}{T_e^{3/2}} \int_{E_c}^{\infty} E(E-3.8)^3 e^{-E/T_e} e^{-0.19(E-3.8)^2} dE \tag{3.10}$$

Where $(1.840411 \times 10^{-11})$ is in the units $cm^3 \cdot eV^{-7/2} \cdot sec^{-1}$. Now let

$$x = E - 3.8 \tag{3.11}$$

Then,

$$\frac{\alpha(T_e)}{No_2} = \frac{(1.840411 \times 10^{-11})}{T_e^{3/2}} e^{-3.8/T_e} \left[\int_0^\infty x^4 e^{-(0.19x^2 + \frac{x}{T_e})} dx + \int_0^\infty x^3 e^{-(0.19x^2 + \frac{x}{T_e})} dx \right] \tag{3.12}$$

The evaluation of the integrals involved in equation (3.12) is found in Appendix C. Applying the results of Appendix C to equation (3.12), one may show that

$$\frac{\alpha(T_e)}{No_2} = c_1 \frac{e^{-3.8/T_e}}{T_e^{3/2}} \left\{ \frac{\sqrt{\pi}}{2} e^{c_2/T_e^2} \operatorname{erfc}\left(\frac{c_3}{T_e}\right) \left[C_4 - \frac{C_5}{T_e} + \frac{C_6}{T_e^2} - \frac{C_7}{T_e^3} + \frac{C_8}{T_e^4} \right] + C_9 - \frac{C_{10}}{T_e} + \frac{C_{11}}{T_e^2} - \frac{C_{12}}{T_e^3} \right\} \tag{3.13}$$

An HP-67 calculator program using a series sum routine was available for computing the erfc function (Ref 5:18-01, L18-01). This program was incorporated into a program for solving equation (3.13). However, the routine overflowed for values of $T_e \leq 0.07$ eV. To preclude this, a small T_e value approximation to equation (3.12) was formulated (Ref 11). Equation (3.12) may be written

$$\frac{\alpha(T_e)}{No_2} = c_1 \frac{e^{-3.8/T_e}}{T_e^{3/2}} \int_0^\infty x^3 e^{-0.19x^2} (x+3.8) e^{-x/T_e} dx \qquad (3.14)$$

For small values of T_e the e^{-x/T_e} term will dominate. Thus,

$$\frac{\alpha(T_e)}{No_2} \simeq c_1 \frac{e^{-3.8/T_e}}{T_e^{3/2}} \int_0^\infty 3.8x^3 e^{-x/T_e} dx \qquad (3.15)$$

Replacing e^{-x/T_e} with 1, the first term in its power series expansion, one may show

$$\frac{\alpha(T_e)}{No_2} \simeq c_{13} T_e^{5/2} e^{-3.8/T_e} \qquad (3.16)$$

The HP-67 program was altered to include equation (3.16). A representative list of $\alpha(T_e)/No_2$ values using both equation (3.13) and the approximation (3.16), and the constants c_1 through c_{13} are in Sppendix D.

It is of interest that the small value approximation for $\alpha(T_e)/No_2$ is about one order of magnitude larger than its exact counterpart (3.13), at $T_e \simeq 1.5$ eV. If, in the final solution of the characteristic value equation (2.65), it is found that the equilibrium T_e is less than about 1.5 eV, then the approximation for $\alpha(T_e)/No_2$ will serve to adequately represent the dissociative attachment rate.

Summary

Using the JILA Report data for dissociative attachment in oxygen,

an analytic representation of the collision cross section $\sigma_d(E)$ was modeled as equation (3.7).

This $\sigma_d(E)$ was used to determine the dissociative attachment rate which is modeled by equation (3.13). Equation (3.16) was postulated to provide a low T_e value approximation to equation (3.13).

This dissociative attachment rate $\alpha(T_e)/No_2$ as a function of T_e may now be used in the three species, three reaction oxygen discharge equation (2.72).

However, it still remains to determine the total ionization rate β as a function of T_e.

IV. The Total Ionization Rate

Finding the functional dependence of the total ionization rate β on the Maxwellian electron temperature T_e, is the final analytic step required to set up the characteristic value problem represented by equations (2.64) and (2.72) for solution. The fact that this ionization rate is also highly dependent on T_e is indicated by its reaction

$$O_2 + e^- \rightarrow O_2^+ + 2e^- \qquad (2.3)$$

Determining the ionization rate β is accomplished in exactly the same manner as determining the dissociative attachment rate (Chapter III). First, an analytic representation for the collision cross section $\sigma_i(E)$ as a function of the electron energy, E, is determined for ionization. Then this result is used in equation (3.4) to determine the analytic representation for the ionization rate.

Cross Section Dependence on Electron Energy

The data used to determine $\sigma_i(E)$ were taken from the JILA Report (Ref 7:106). The threshold energy for ionization E_i is 12.063 eV. Because of this relatively high E_i and because the bell-shaped data curve does not begin to bend over until the electron energy is over 100 eV, it was deemed adequate to only model the lower portion of the forward edge of the data curve. The data points are in Figure 4-1. For comparison, the data curve for dissociative attachment (Fig. 3-1) is represented on Figure 4-1 by the small triangle to the left of the origin.

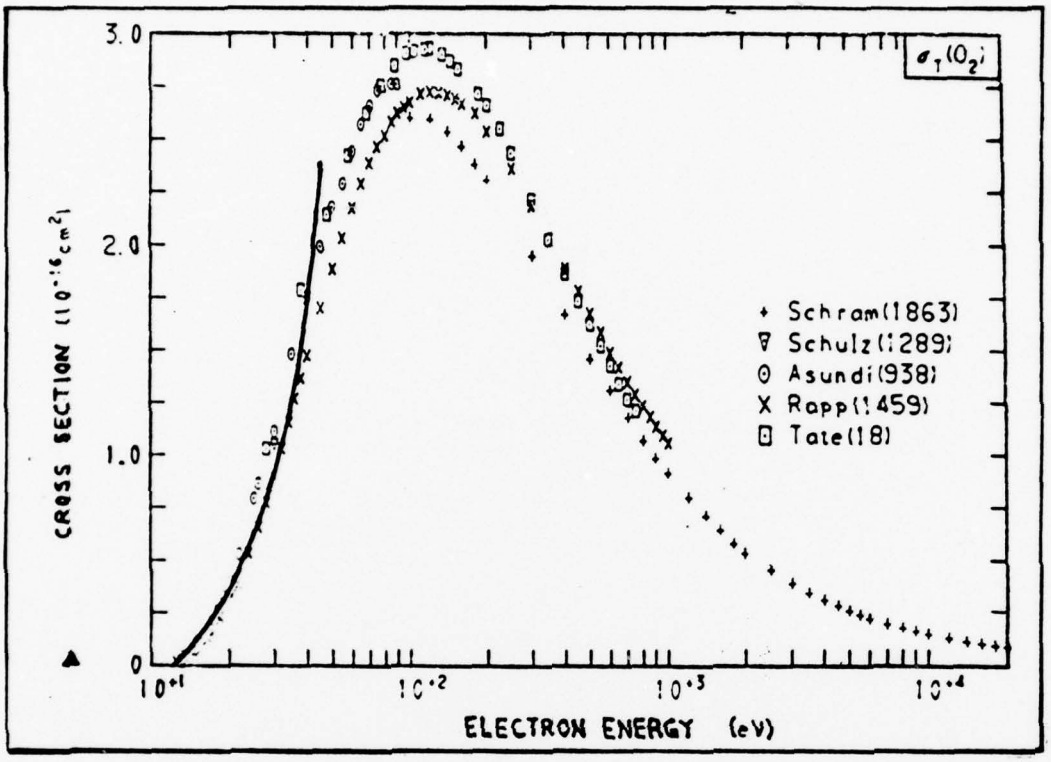

Figure 4-1. Data and Analytic Curve for Total Ionization Cross Sections vs. Electron Energy in Oxygen (Ref 7:106)

Using the HP-67 "Curve Fitting" program (Ref 6:03-01, L03-01) to establish an initial representation of $\sigma_i(E)$ and then iterating the constants involved, the final analytic representation was found to be

$$\sigma_i(E) = (4.0\text{x}10^{-17})e^{0.045E} - (6.8835145\text{x}10^{-17}) \qquad (4.1)$$

Where $\sigma_i(E)$ is in cm^2, E is in eV^{-1}, the constants $(4.0\text{x}10^{-17})$ and $(6.8835145\text{x}10^{-17})$ in cm^2, and the constant 0.045 in eV^{-1}. The analytic curve $\sigma_i(E)$, (4.1), represents the data well up to about 30 eV. Figure 4-1 shows the data and the analytic curve $\sigma_i(E)$.

Determination of $\beta(T_e)/No_2$

The ionization rate $\beta(T_e)/No_2$ is determined in exactly the same fashion as the dissociative attachment rate. Analogous to equation (3.8) is

$$\frac{\beta(T_e)}{No_2} = \int_{E_i}^{\infty} \left[(4.0\times10^{-17})e^{0.045E} - (6.8835145\times10^{-17})\right] \frac{2}{\sqrt{\pi}} T_e^{-3/2} E^{1/2} e^{-E/T_e} \left(\frac{2E^*}{m_e}\right)^{1/2} dE \tag{4.2}$$

Collecting the constants in front of the integral and rearranging, one may write the equation as

$$\frac{\beta(T_e)}{No_2} = \frac{a}{T_e^{3/2}} \int_{E_i}^{\infty} Ee^{cE} e^{-E/T_e} dE - \frac{b}{T_e^{3/2}} \int_{E_i}^{\infty} Ee^{-E/T_e} dE \tag{4.3}$$

where

$$a = 2.6769\times10^{-9} \quad eV^{3/2} \quad cm^3 \quad sec^{-1} \tag{4.4}$$

$$b = 4.6067\times10^{-9} \quad eV^{-1/2} \quad cm^3 \quad sec^{-1} \tag{4.5}$$

$$c = 0.045 \quad eV^{-1} \tag{4.6}$$

$$E_i = 12.063 \quad eV \tag{4.7}$$

By letting $x = E-E_i$ and carrying out the integration, it may be shown that

$$\frac{\beta(T_e)}{No_2} = \frac{ae^{-E_i\left(\frac{1}{T_e}-c\right)}}{T_e^{3/2}} \left[\frac{1}{\left(\frac{1}{T_e}-c\right)}\right]\left[\frac{1}{\left(\frac{1}{T_e}-c\right)} + E_i\right] - bE^{-E_i/T_e}\left[T_e^{1/2}+E_iT_e\right]^{-1/2} \tag{4.8}$$

Some representative rates for $\beta(T_e)/No_2$ are tabulated and compared to $\alpha(T_e)/No_2$ in Appendix D.

Summary

An analytic model of the collision cross section for total ionization as a function of electron energy $\sigma_i(E)$ has been postulated. This collision cross section has been used to determine an analytic representation of the total ionization rate as a function of the electron temperature T_e. Using $\beta(T_e)/No_2$ as well as the previously determined $\alpha(T_e)/No_2$, it is possible to compute numerical results for the three species, three reaction oxygen discharge that was modeled as the characteristic value problem (2.64) and (2.72).

V. Numerical Results for the Three Species, Three Reaction Oxygen Discharge

The characteristic value problem, equations (2.64) and (2.72), is now solved by using the results from Chapter III and Chapter IV which provided the models for the dissociative attachment rate $\alpha(T_e)/No_2$ and for the ionization rate $\beta(T_e)/No_2$.

Method of Solution

The system of equations used to compute numerical results is

$$\frac{J_-}{N_e} = \frac{2\sigma_i^2 T_o \alpha - \beta\gamma m_+ \nu_+ + \sigma_i^2 T_e \gamma}{2\sigma_i^3 T_o + \gamma\sigma_i m_- \nu_-} \tag{2.68}$$

$$\frac{N_-}{N_e} = \frac{\alpha}{\gamma} + \frac{\sigma_i}{\gamma}\left(\frac{J_-}{N_e}\right) \tag{2.70}$$

$$\frac{J_e}{N_e} = \frac{\beta}{\sigma_i} - \left(\frac{J_-}{N_e}\right) \tag{2.71}$$

$$\sigma_i m_e \nu_e \left(\frac{J_-}{N_e}\right)^2 + \left[\sigma_i^2(T_e - T_o) - m_e\nu_e(\alpha+\beta) - \gamma m_- \nu_-\right]\left(\frac{J_-}{N_e}\right)$$

$$+ \left[\frac{\alpha\beta}{\sigma_i} m_e \nu_e - \sigma_i \alpha (T_e - T_o)\right] = F(T_e) \tag{2.72}$$

An HP-67 program was written to evaluate $\frac{J_-}{N_e}$, $\frac{J_e}{N_e}$, $\frac{N_-}{N_e}$, and $F(T_e)$. T_e was adjusted to find $F(T_e) = 0$. The program was initialized by inputting the dissociative attachment rate, $\alpha(T_e)/No_2$, and the total ionization rate, $\beta(T_e)/No_2$.

$F(T_e)$ was calculated using equation (2.72) for a range of T_e's from 0.1 eV to 20 eV (see Appendix D for a sample list of values obtained by this method). By observing the zero crossings made by $F(T_e)$, it was possible to establish equilibrium T_e candidates. Then $F(T_e)$ was iterated around these T_e values in order to further refine the equilibrium temperature.

The number density ratio N_-/N_e was used as the criterion for eliminating non-physical equilibrium T_e values. Since the ratio N_-/N_e must be a positive quantity, any equilibrium T_e values which had an associated negative number density ratio N_-/N_e were discarded.

In order numerically to solve the characteristic value problem, it was necessary to know the values of the constants σ_1, T_o, $m_e\nu_e$, $m_-\nu_-$, $m_+\nu_+$, and the detachment rate γ.

Constants Used in the Solution

The final solution of the model requires that the values of the constants in equations (2.68), (2.70), (2.71), and (2.72) be established.

The radius of the discharge tube was assumed to be 1.1 cm (Ref 3). This established the constant in the Bessel function argument, $J_o(\sigma_1 r)$ and $J_1(\sigma_1 r)$, as

$$\sigma_1 = 2.1862 \text{ cm}^{-1} \tag{5.1}$$

The background gas temperature, T_o, was assumed to be

$$T_o = 300°K \tag{5.2}$$

In order to establish values for the dissociative attachment rate $\alpha(T_e)$ and the total ionization rate $\beta(T_e)$, it was necessary to determine at what O_2 background gas pressures the discharge would be operated.

It was desired to make a comparison with Sabadil's numerical solution of the three species, three reaction oxygen discharge; therefore, it was decided to simulate the discharge at pressures of 0.2 torr, 0.5 torr, 1.0 torr (Ref 17:235-251). 5.0 torr was also included.

Sabadil uses electric field to pressure ratios, E/p in volt·cm^{-1}/torr, of 40, 30, and 20 for the operating pressures of 0.2, 0.5, and 1.0 torr, respectively (Ref 17:240). Using the same E/p values, it was possible to determine the mobilities μ_λ for the three different species, with the mobility relation

$$\mu_\lambda = \frac{q_o}{m_\lambda \nu_\lambda} \tag{5.3}$$

McDaniel and Mason give a complete set of mobility vs. E/p curves for the ionic species in background O_2 at 300°K (Ref 12:292-293). These curves were used to determine the values of $m_-\nu_-$ and $m_+\nu_+$ at all the operating pressures considered. Sabadil's electron mobility values for electrons in O_2 at 300°K were used to determine $m_e\nu_e$ for operating pressures of 0.2 torr, 0.5 torr, and 1.0 torr (Ref 17:240). Using Brown's data for the electron drift speed vs. E/p and the drift speed mobility relation $v_d = \mu_\lambda E$, it was possible to determine the value of $m_e\nu_e$ at a pressure of 5.0 torr (Ref 1:57).

The final constant required before beginning a numerical calculation was the detachment rate γ, determined by the reaction

$$O^- + O \rightarrow O_2 + e^- \tag{2.2}$$

It was assumed that γ was equal to the atomic oxygen number density multiplied by an appropriate rate. Garscadden suggested that at equilibrium the atomic oxygen, O, concentration was about 3% of the molecular O_2 concentration (Ref 3). An appropriate rate for the

reaction was taken from Dettmer's dissertation (Ref 2:263). Thus,

$$\gamma = (0.03\ No_2)(1.9x10^{-10} cm^3 \cdot sec^{-1}) \qquad (5.3)$$

Table VI in Appendix D contains a list of all the constants used for the solution of the characteristic value problem (2.72).

Results

The results from the solution of the three species, three reaction oxygen discharge model are displayed in Table I.

Table I

Three Species, Three Reaction Model Results

Pressure in torr	Equilibrium T_e eV	N_-/N_e	J_-/N_e in cm/sec	J_e/N_e in cm/sec	J_-/J_e
0.2	3.67	1.31 02	-2.09 06	3.14 06	-6.65 -01
0.5	2.21	1.29 01	-3.41 05	5.22 05	-6.52 -01
1.0	1.50	2.26	-2.33 04	4.25 04	-5.48 -01
5.0	0.99	4.59 -01	-5.18 02	1.71 03	-3.03 -01

The reaction rates at these equilibrium T_e's are displayed in Table II. The negative sign on the ratio J_-/N_e indicates that the O^- ions are diffusing radially inward. It should be noted that if one assumes that J_1/J_o is approximately equal to 1, the radial diffusion speed of the electrons is given by J_e/N_e. Dividing J_-/N_e by N_-/N_e, the approximate radial diffusion speed for the O^- ions may be found (see equation (2.79). Graphic results are on the following pages.

Table II

Equilibrium Reaction Rates for the Three Species, Three Reaction Model

Pressure in torr	Equilibrium T_e eV	$\alpha(T_e)$ in sec^{-1}	$\beta(T_e)$ in sec^{-1}	γ in sec^{-1}
0.2	3.67	2.46 05	2.31 06	2.67 04
0.5	2.21	4.03 05	3.98 05	9.17 04
1.0	1.50	3.63 05	4.20 04	1.83 05
5.0	0.99	4.20 05	2.61 03	9.17 05

Summary

The postulated model of the three species, three reaction oxygen discharge has produced single equilibrium temperatures which are associated with physically consistent values of number densities and of fluxes.

Figure 5-1 indicates that the electron temperature T_e at equilibrium decreases with increasing pressure. It may perhaps be extended to indicate that for discharge pressures greater than 5 torr the equilibrium electron temperature may essentially become constant around 1 eV.

Figure 5-2 indicates that the number density ratio N_-/N_e also decreases with increasing pressure; and at pressures below about 1 torr the number of O^- ions significantly outnumbers the electrons.

Figure 5-3 indicates that the radial diffusion current densities, J_- and J_e are both inversely proportional to the discharge pressure, but that the O^- current density decreases faster with pressure than the electron current density.

In Figure 5-4 the curve for the dissociative attachment rate α, indicates that over the pressure range considered the production of O^- ions is saturated.

The O^- ions are diffusing radially inward toward the axis of the discharge tube. This result concurs with that of Sabadil (Ref 17:235).

It should be noted that the method of solution used mobilities to define $m_-\nu_-$ and $m_+\nu_+$. These mobilities are actually functions of E/p. In order to achieve a closed solution, it may be necessary to iterate the entire solution based on the equilibrium electric field E_o from equation (2.72) until it agrees with the electric field used to determine the mobilities.

The primary result has been to show that Lee's method for attaining a solution to the three species, three reaction oxygen discharge leads to physically consistent results in some cases and has possibilities for extension to more than three species (Ref 10:1-7).

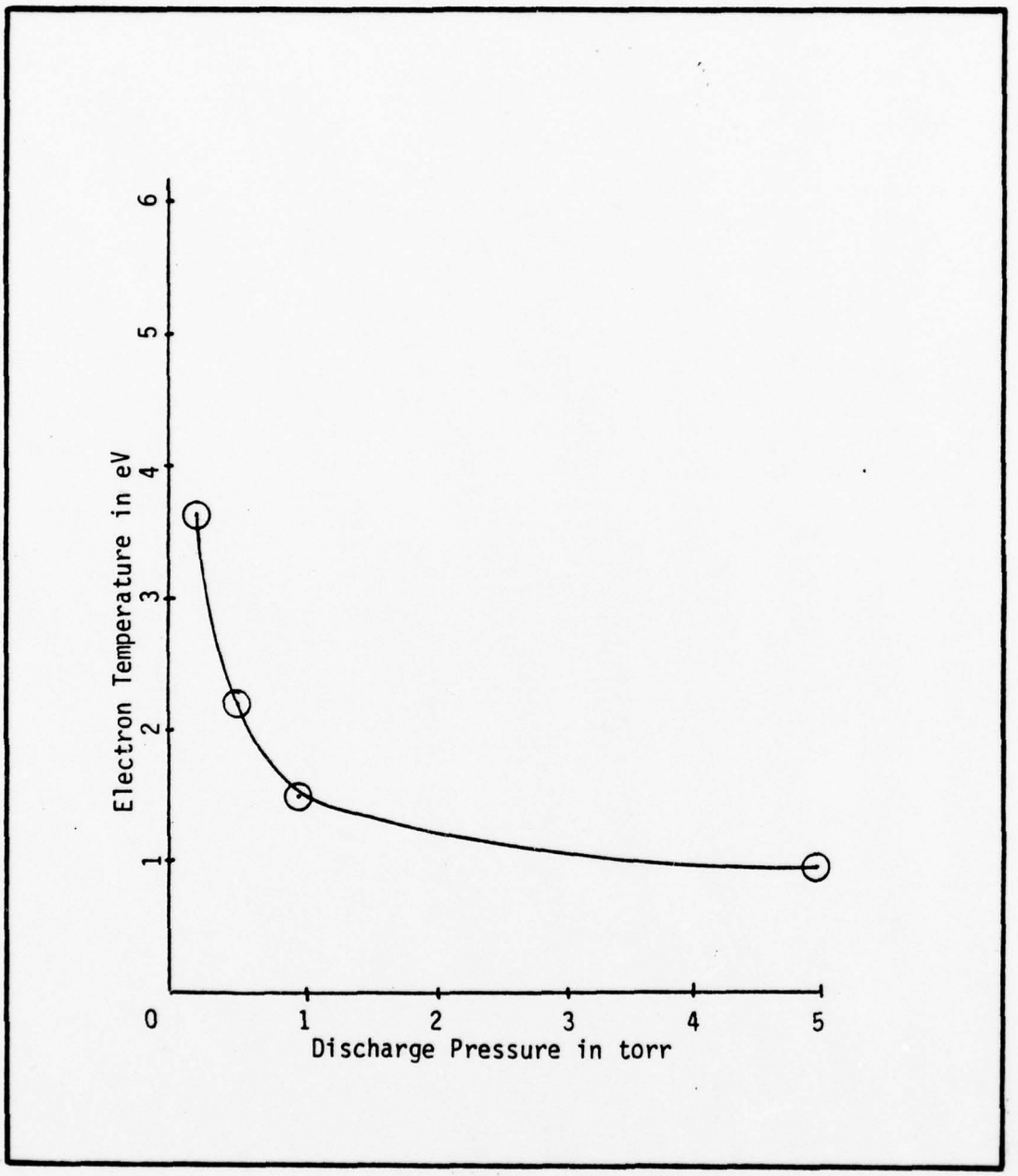

Figure 5-1. Equilibrium Electron Temperature vs. Pressure for the Three Species Model

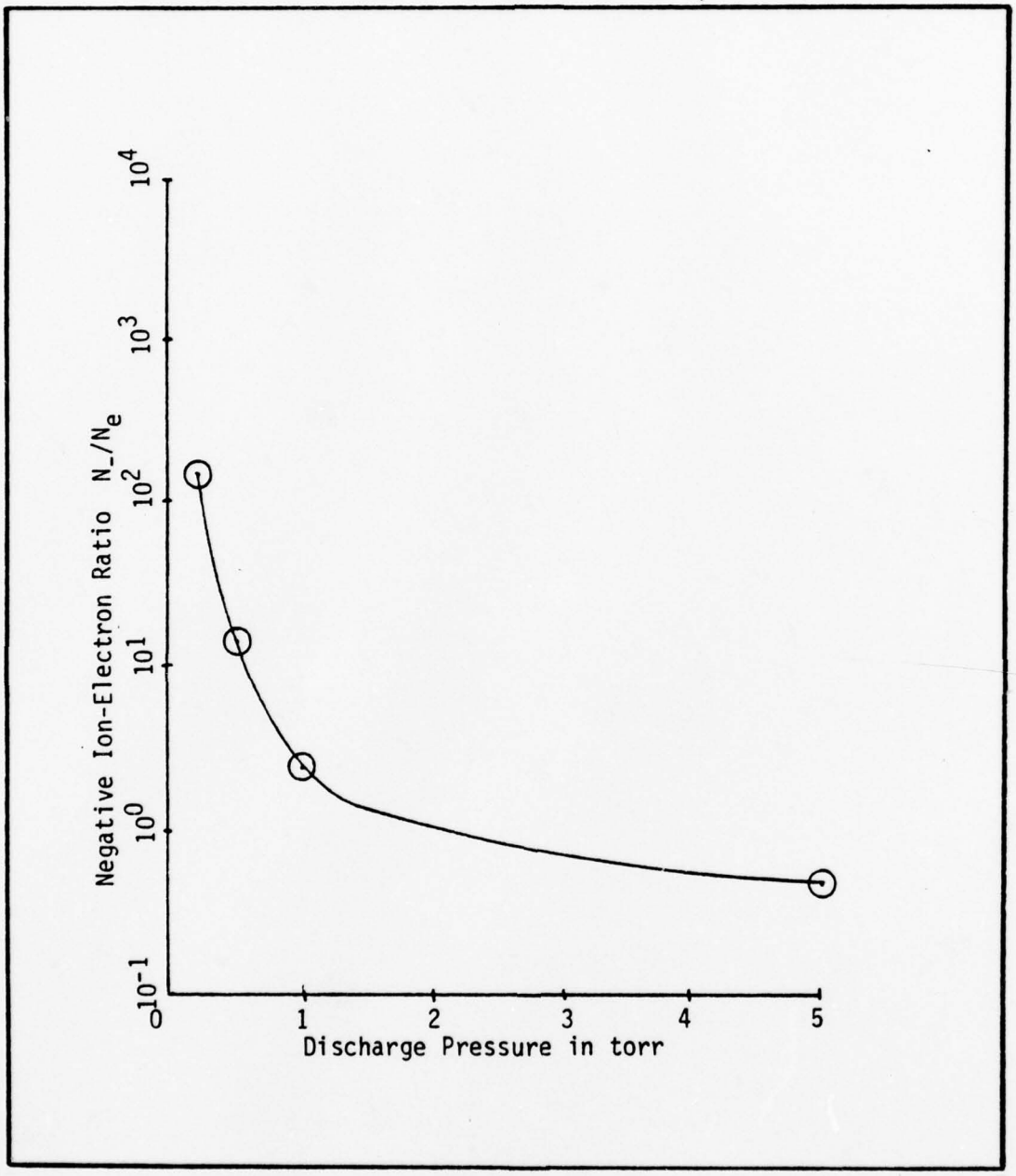

Figure 5-2. Equilibrium N_-/N_e vs. Pressure for the Three Species Model

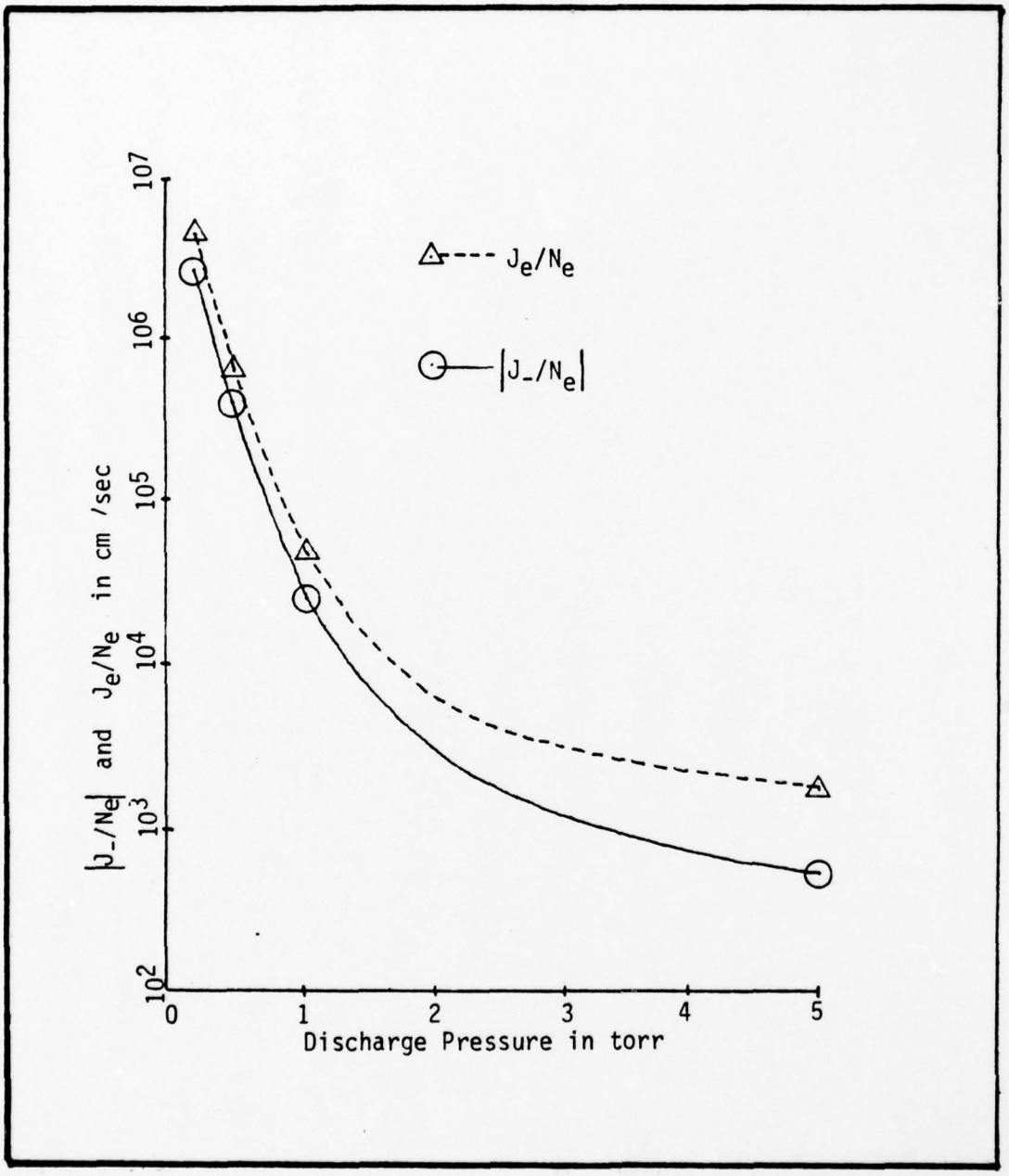

Figure 5-3. Equilibrium Radial Current Density Ratios vs. Pressure in the Three Species Model

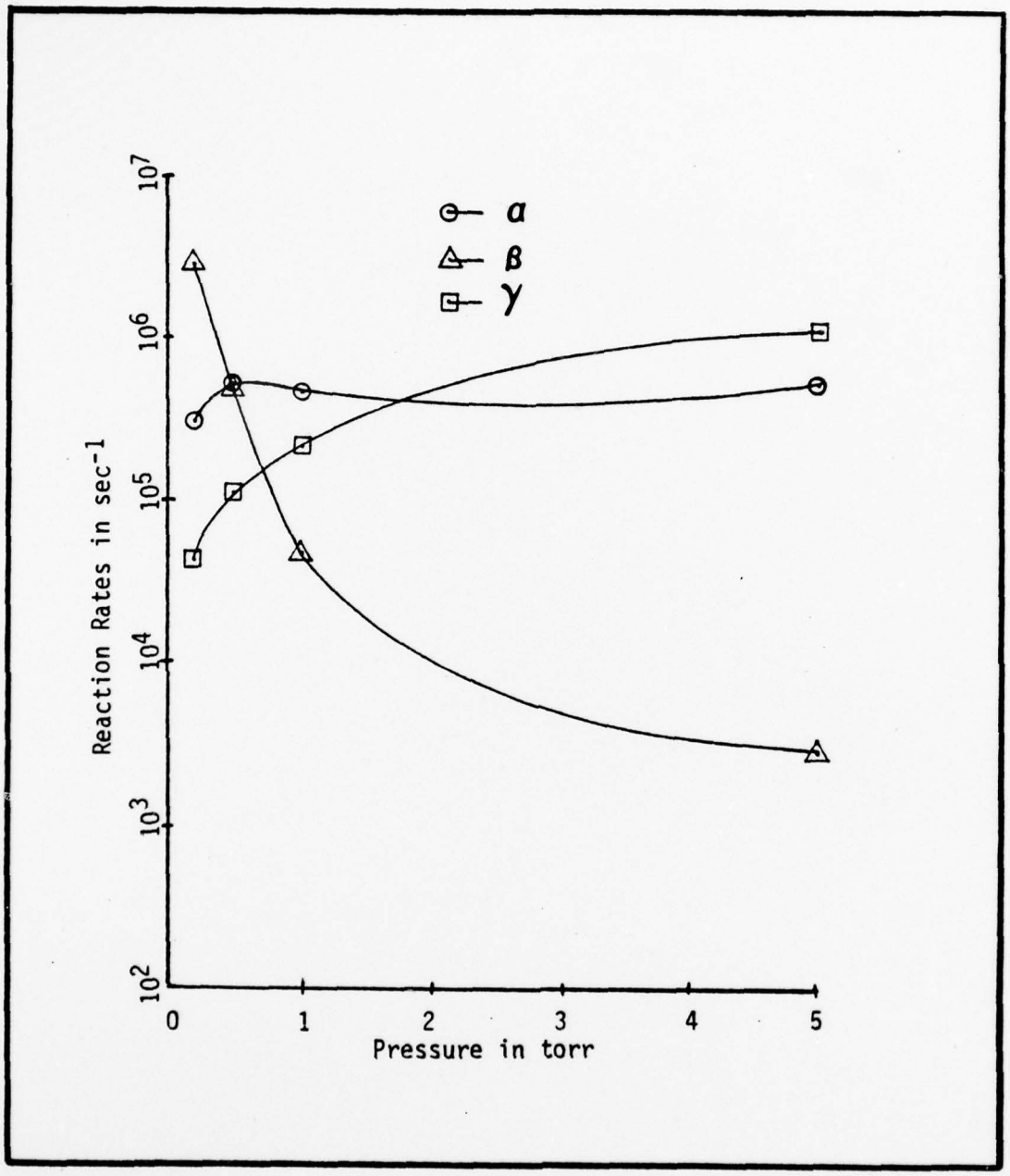

Figure 5-4. Equilibrium Reaction Rates vs. Pressure for the Three Species, Three Reaction Model

VI. An Equilibrium Model for the Four Species, Four Reaction Oxygen Discharge

The method used for solving the three species, three reaction oxygen discharge may be utilized to solve the four species, four reaction oxygen discharge. The new species is the negative oxygen molecule O_2^-. It is produced by the charge transfer reaction.

$$O_2 + O^- \rightarrow O_2^- + O \tag{6.1}$$

The reaction rate associated with this reaction is δ.

An extra reaction and ion do not significantly alter the method of solution previously outlined. Therefore, only the cogent differences will be outlined here before displaying the form of the characteristic value problem.

Solution

The specific moment equations for the system are the particle conservation equations

$$j_e' + {}^{j_e}/_r = (\beta-\alpha)n_e + \gamma n_- \tag{6.2}$$

$$j_-' + {}^{j_-}/_r = \alpha n_e - (\gamma+\delta)n_- \tag{6.3}$$

$$j_+' + {}^{j_+}/_r = \beta n_e \tag{6.4}$$

$$j_{2-}' + {}^{j_{2-}}/_r = \delta n_- \tag{6.5}$$

The radial momentum conservation equations are

$$j_e + \frac{-T_e}{m_e \nu_e} n_e' - \frac{q_o}{m_e \nu_e} n_e E_r \tag{6.6}$$

$$j_- = \frac{-To}{m_-\nu_-} n_-' - \frac{q_o}{m_-\nu_-} n_- E_r \tag{6.7}$$

$$j_+ = \frac{-T_o}{m_+\nu_+} n_+' + \frac{q_o}{m_+\nu_+} n_+ E_r \tag{6.8}$$

$$j_{2-} = \frac{-T_o}{m_{2-}\nu_{2-}} n_2' - \frac{q_o}{m_{2-}\nu_{2-}} n_{2-} E_r \tag{6.9}$$

The axial momentum equations are

$$u_e = \frac{-q_o}{m_e\nu_e} E_o \tag{6.10}$$

$$u_- = \frac{-q_o}{m_-\nu_-} E_o \tag{6.11}$$

$$u_+ = \frac{q_o}{m_+\nu_+} E_o \tag{6.12}$$

$$u_{2-} = \frac{-q_o}{m_{2-}\nu_{2-}} E_o \tag{6.13}$$

The energy equation is

$$T_e = \frac{m_e\nu_e u_e^2}{\nu_{eo}} \tag{6.14}$$

And Poisson's equation is used to close the system:

$$E_r' + \frac{E_r}{r} = \frac{q_o}{\epsilon_o}(n_+ - n_e - n_- - n_{2-}) \tag{6.15}$$

It is assumed that the O_2^- ions are at the same temperature as the background O_2. The subscript $_{2-}$ identifies parameters associated with the O_2^- ion.

To eliminate the radial electric field, E_r, the following identities may be used

$$n_- n_e E_r = n_e n_- E_r \tag{6.16}$$

$$n_{2-} n_e E_r = n_e n_{2-} E_r \tag{6.17}$$

$$n_{2-} n_- E_r = n_- n_{2-} E_r \tag{6.18}$$

The system can be reduced to the six equations

$$j_e' + {}^{j_e}/_r = (\beta-\alpha) n_e + \gamma n_- \tag{6.19}$$

$$j_-' + {}^{j_-}/_r = \alpha n_e - (\gamma+\delta) n_- \tag{6.20}$$

$$j_{2-}' + {}^{j_{2-}}/_r = \delta n_- \tag{6.21}$$

$$j_e(m_+\nu_+ + m_e\nu_e) + j_-(m_+\nu_+ + m_-\nu_-) + j_{2-}(m_+\nu_+ + m_{2-}\nu_{2-}) = -n_e'(T_e+T_o)$$

$$-2T_o n_-' - 2T_o n_{2-}' \tag{6.22}$$

$$T_o n_-' n_{2-} + m_-\nu_- j_- n_{2-} = T_o n_{2-}' n_- + m_{2-}\nu_{2-} j_{2-} n_- \tag{6.23}$$

$$T_o(n_- + n_{2-}) n_e' + m_e\nu_e j_e (n_- + n_{2-}) = T_o (n_- + n_{2-})' n_e$$

$$+ n_e (m_-\nu_- j_- + m_{2-}\nu_{2-} j_{2-}) \tag{6.24}$$

The boundary conditions are

$$n_e'(0) = n_-'(0) = n_{2-}'(0) = 0 \tag{6.25}$$

$$n_e(R) = n_-(R) = n_{2-}(R) = 0 \tag{6.26}$$

Using an extension of Lee's magic substitutions, (2.54) and (2.55), the system becomes

$$\begin{pmatrix} 0 & -\sigma_1 & 0 & 0 \\ 0 & 0 & -\sigma_1 & 0 \\ 0 & 0 & 0 & -\sigma_1 \\ 2\sigma_1 T_0 - (m_+\nu_+ + m_e\nu_e) & -(m_+\nu_+ + m_-\nu_-) & -(m_+\nu_+ + m_{2-}\nu_{2-}) & \end{pmatrix} \begin{pmatrix} \frac{N_{2-}}{N_e} \\ \frac{J_e}{N_e} \\ \frac{J_-}{N_e} \\ \frac{J_{2-}}{N_e} \end{pmatrix} = \begin{pmatrix} \alpha - \beta \\ -\alpha \\ 0 \\ -\sigma_1(T_e + T_0) \end{pmatrix} + \frac{N_-}{N_e} \begin{pmatrix} -\gamma \\ \gamma + \delta \\ -\delta \\ -2\sigma_1 T_0 \end{pmatrix} \tag{6.27}$$

plus the non-linear equations

$$m_-\nu_-\left(\frac{N_{2-}}{N_e}\right)\left(\frac{J_-}{N_e}\right) = m_{2-}\nu_{2-}\left(\frac{N_-}{N_e}\right)\left(\frac{J_{2-}}{N_e}\right) \tag{6.28}$$

$$\left[\frac{N_-}{N_e} + \frac{N_{2-}}{N_e}\right]\left[\sigma_1(T_0 - T_e) + m_e\nu_e\left(\frac{J_e}{N_e}\right)\right] - m_-\nu_-\left(\frac{J_-}{N_e}\right) - m_{2-}\nu_{2-}\left(\frac{J_{2-}}{N_e}\right) = 0 \tag{6.29}$$

Equation (6.27) is solved for the ratios $\frac{N_{2-}}{N_e}$, $\frac{J_e}{N_e}$, $\frac{J_-}{N_e}$, and $\frac{J_{2-}}{N_e}$, in terms of the ratio $\frac{N_-}{N_e}$. Then equation (6.28) is solved for the ratio $\frac{N_-}{N_e}$. Equation (6.29) is the characteristic value equation for computing the equilibrium T_e's.

Solving equation (6.27) one finds that

$$\begin{pmatrix} \frac{N_{2-}}{N_e} \\ \frac{J_e}{N_e} \\ \frac{J_-}{N_e} \\ \frac{J_{2-}}{N_e} \end{pmatrix} = \underset{\sim}{R}(T_e) + \underset{\sim}{S}(T_e)\frac{N_-}{N_e} \tag{6.30}$$

Where

$$\begin{pmatrix} -\frac{T_e}{2T_o} + \frac{\alpha m_- \nu_- + \beta m_+ \nu_+}{2\sigma_i^2 T_o} \\ \frac{\beta-\alpha}{\sigma_i} \\ \frac{\alpha}{\sigma_i} \\ 0 \end{pmatrix} = \underset{\sim}{R}(T_e) = \begin{pmatrix} R_1 \\ R_2 \\ R_3 \\ R_4 \end{pmatrix} \tag{6.31}$$

and

$$\begin{pmatrix} \frac{\delta m_{2-}\nu_{2-} - m_{-}\nu_{-}(\gamma+\delta)}{2\sigma_i^2 T_o} - 1 \\ \frac{\gamma}{\sigma_i} \\ \frac{-(\gamma+\delta)}{\sigma_i} \\ \frac{\delta}{\sigma_i} \end{pmatrix} = \underset{\sim}{S}(T_e) = \begin{pmatrix} S_1 \\ S_2 \\ S_3 \\ S_4 \end{pmatrix} \tag{6.32}$$

It has been assumed that $T_e >> T_o$ and $m_{-}\nu_{-} >> m_e\nu_e$. Then the solution of the four species, four reaction oxygen discharge is the following set of equations:

$$\left[\frac{N_-}{N_e}\right]_- = \frac{-L - \sqrt{L^2-4KM}}{2K} \; ; \left[\frac{N_-}{N_e}\right]_+ = \frac{-L + \sqrt{L^2-4KM}}{2K} \tag{6.33}$$

Where,

$$K = m_{-}\nu_{-}S_1S_3 - m_{2-}\nu_{2-}S_4 \tag{6.34}$$

$$L = m_{-}\nu_{-}(R_1S_3+S_1R_3) \tag{6.35}$$

$$M = m_{-}\nu_{-}R_1R_3 \tag{6.36}$$

Where,

$$R_1 = \frac{-T_e}{2T_o} + \frac{\alpha m_{-}\nu_{-} + \beta m_{+}\nu_{+}}{2\sigma_i^2 T_o} \tag{6.37}$$

$$R_2 = \frac{\beta-\alpha}{\sigma_i} \tag{6.38}$$

$$R_3 = \frac{\alpha}{\sigma_1} \tag{6.39}$$

$$S_1 = \frac{\delta m_{2-} \nu_{2-} - m_- \nu_- (\gamma+\delta)}{2\sigma_1^2 T_o} - 1 \tag{6.40}$$

$$S_2 = \frac{\gamma}{\sigma_1} \tag{6.41}$$

$$S_3 = \frac{-(\gamma+\delta)}{\sigma_1} \tag{6.42}$$

$$S_4 = \frac{\delta}{\sigma_1} \tag{6.43}$$

Now,

$$\frac{N_{2-}}{N_e} = R_1 + S_1\left[\frac{N_-}{N_e}\right]_{\pm} \tag{6.44}$$

$$\frac{J_e}{N_e} = R_2 + S_2\left[\frac{N_-}{N_e}\right]_{\pm} \tag{6.45}$$

$$\frac{J_-}{N_e} = R_3 + S_3\left[\frac{N_-}{N_e}\right]_{\pm} \tag{6.46}$$

$$\frac{J_{2-}}{N_e} = R_4 + S_4\left[\frac{N_-}{N_e}\right]_{\pm} \tag{6.47}$$

And the characteristic value equation for T_e is

$$\left[\frac{N_-}{N_e} + \frac{N_{2-}}{N_e}\right]\left[-\sigma_1 T_e + m_e \nu_e \left(\frac{J_e}{N_e}\right)\right] - m_- \nu_- \left(\frac{J_-}{N_e}\right) - m_{2-} \nu_{2-} \left(\frac{J_{2-}}{N_e}\right) = F(T_e) = 0 \tag{6.48}$$

It may be observed from equation (6.33) that the number density ratio $\frac{N_-}{N_e}$ has two values. This is due to the fact that $\frac{N_-}{N_e}$ is the root of the quadratic equation (6.28). Therefore, the characteristic value equation (6.48) must be evaluated for both the $\left[\frac{N_-}{N_e}\right]_-$ and the $\left[\frac{N_-}{N_e}\right]_+$ roots for a single test T_e.

A program was written for the HP-67 that computed $F(T_e)$ for both $\left[\frac{N_-}{N_e}\right]_-$ and $\left[\frac{N_-}{N_e}\right]_+$ and yielded the ratios $\frac{N_{2-}}{N_e}$, $\frac{J_e}{N_e}$, $\frac{J_-}{N_e}$, and $\frac{J_{2-}}{N_e}$. Using this program, it was possible to begin searching for the equilibrium T_e.

Numerical Results

In order to solve the characteristic value problem represented by equation (6.48), it was necessary to determine the rate δ for the reaction

$$O^- + O_2 \rightarrow O_2^- + O \qquad (6.1)$$

Harrison and Moruzzi have investigated this reaction rate, δ, as a function of E/p (Ref 4:1244). Their results were used for interpolation to the lower E/p values required for this model, i.e., 40, 30, 20, and 10. The reaction rate δ's used are listed in Appendix D along with all of the other constants necessary for the solution of equation (6.48).

The results of the computation for the four species, four reaction oxygen discharge model are listed in Table III and Table IV.

Table III

Four Species, Four Reaction Results

Pressure in torr	Equilibrium T_e in e_V	N_-/N_e	N_2/N_e	J_e/N_e in cm/sec	J_-/N_e in cm/sec	J_{2_-}/N_e in cm/sec
0.2	5.51	3.77	5.48 03	5.28 06	7.72 01	4.99 04
0.5	4.15	5.25	1.15 04	4.38 06	6.65 01	6.91 04
1.0	3.54	5.88	2.12 04	4.22 06	3.28 01	6.06 04
5.0	2.59	5.11	1.11 05	4.52 06	5.92	8.11 04

Table IV

Equilibrium Reaction Rates for the
Four Species, Four Reaction Model

Pressure in torr	Equilibrium T_e in e_V	α in sec^{-1}	β in sec^{-1}	γ in sec^{-1}	δ in sec^{-1}
0.2	5.51	2.48 05	1.66 07	3.67 04	2.90 04
0.5	4.15	6.33 05	9.74 07	9.17 04	2.90 04
1.0	3.54	1.21 06	9.56 06	1.83 05	2.25 04
5.0	2.59	4.88 06	1.06 07	9.17 05	3.70 04

Again, by assuming that $\frac{J_1}{J_o}$ is approximately 1, the radial diffusion speeds of the electrons and of the negative ions may be approximated by using the values in Table III and equation (2.79).

The results are displayed graphically on the following pages.

Summary

Again, the postulated model has produced single equilibrium temperatures, T_e. They were regarded as physically consistent because neither of the two number density ratios, N_-/N_e or N_{2-}/N_e, was negative. Secondarily, these T_e values produce other physically plausable discharge parameters.

Figure 6-1 indicates that the electron temperature decreases with increasing pressure. This may be due to the fact that increasing the pressure reduces the radial diffusion to the tube wall; therefore, the loss rates of charged species is reduced. Then the available electron energy must be distributed over more electrons, and the average electron temperature thus is decreased. Also, if one assumes that the electric field varies only slowly with pressure, the electrons have shorter paths over which to be accelerated at the higher pressures.

Figure 6-2 indicates that at all pressures considered, negative ions outnumber electrons. But now it appears that the dominant ion is the O_2^-. In all cases it far exceeds the meagre supply of O^- ions in the discharge. The number of O^- remains fairly constant over the pressures considered, but the number of O_2^- ions increases with increasing pressure. Thus, it may be concluded that the charge transfer reaction (6.1), which produces the O_2^- ion, is the dominate reaction. This conclusion does not agree with the experimental observation that the O^- ion is more numerous than the O_2^- ion.

Figure 6-3 indicates that the radial diffusion current densities J_e/N_e, J_-/N_e, and J_{2-}/N_e remain relatively constant as the discharge pressure is increased. Only the O^- ion current density decreases slowly with increasing pressure.

Figure 6-4 indicates that as the pressure increases the dissociative attachment rate, α, increases. This is due to its dependence on T_e and the neutral species density. The ionization rate, β, initially decreases but then remains fairly constant over the range of pressures considered. Since the detachment rate, γ, is modeled as being directly proportional to the pressure, it increases as the pressure is raised. The charge transfer reaction rate, δ, remains fairly constant as the pressure increases.

In this model, the electrons and positive and negative ions are all diffusing outward toward the tube wall under the conditions postulated. This indicates that the outward radial flux of the negative particles balances the outward radial flux of the positive ions. This result is supported by the higher production rate of positive ions in the four species model than in the three species model.

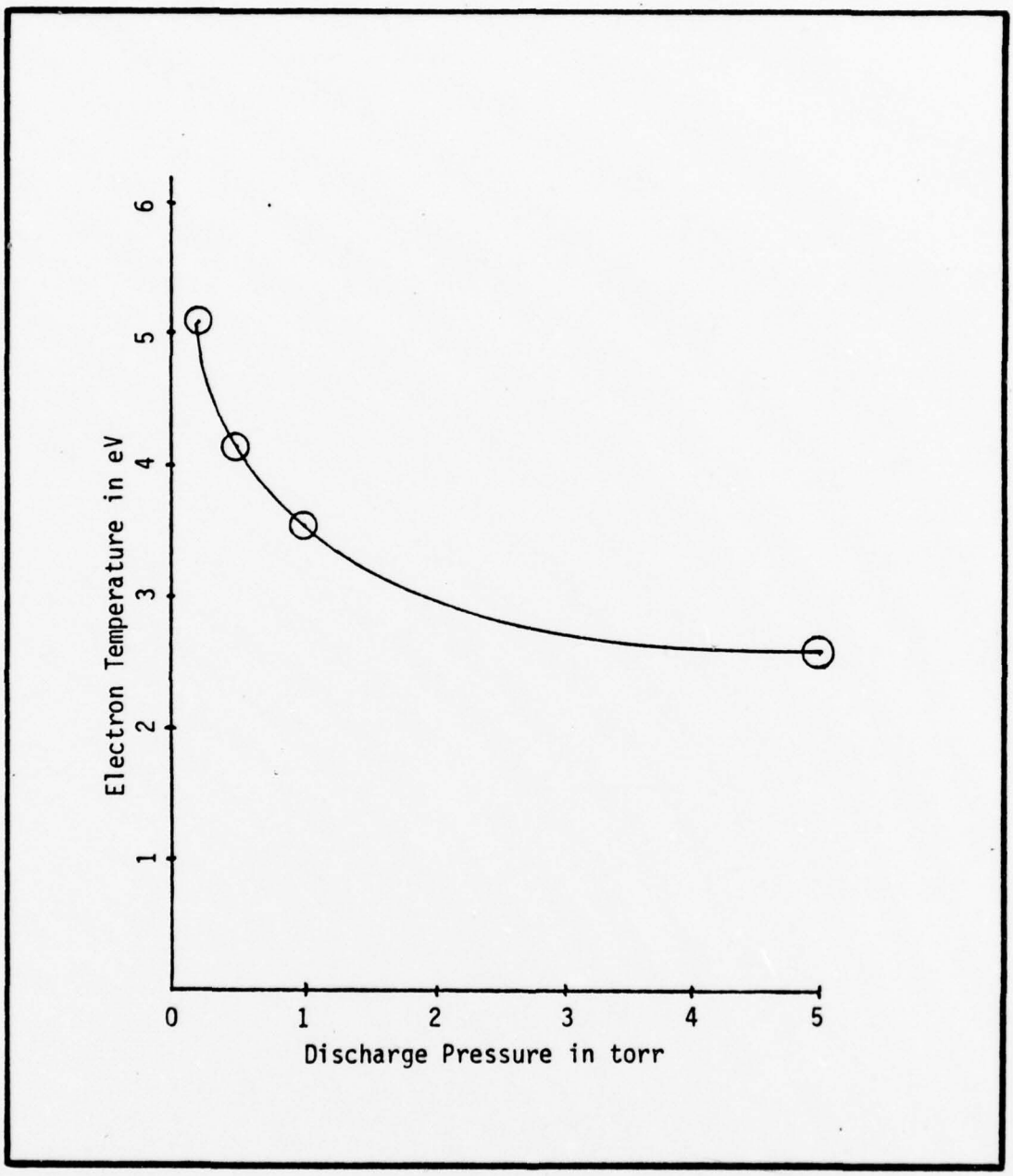

Figure 6-1. Equilibrium Electron Temperature vs. Pressure for the Four Species, Four Reaction Model

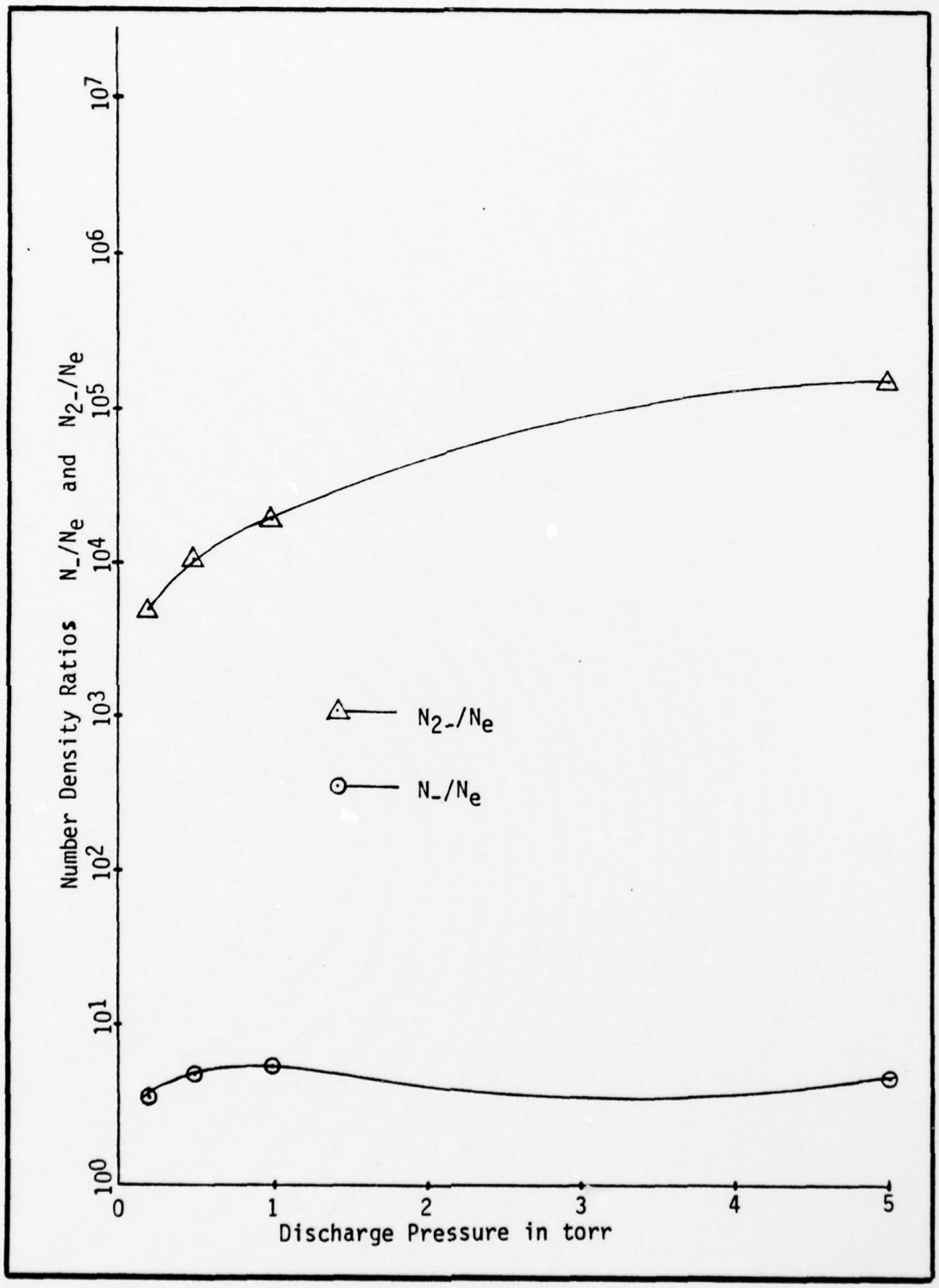

Figure 6-2. Equilibrium Number Density Ratios vs. Pressure for the Four Species, Four Reaction Model

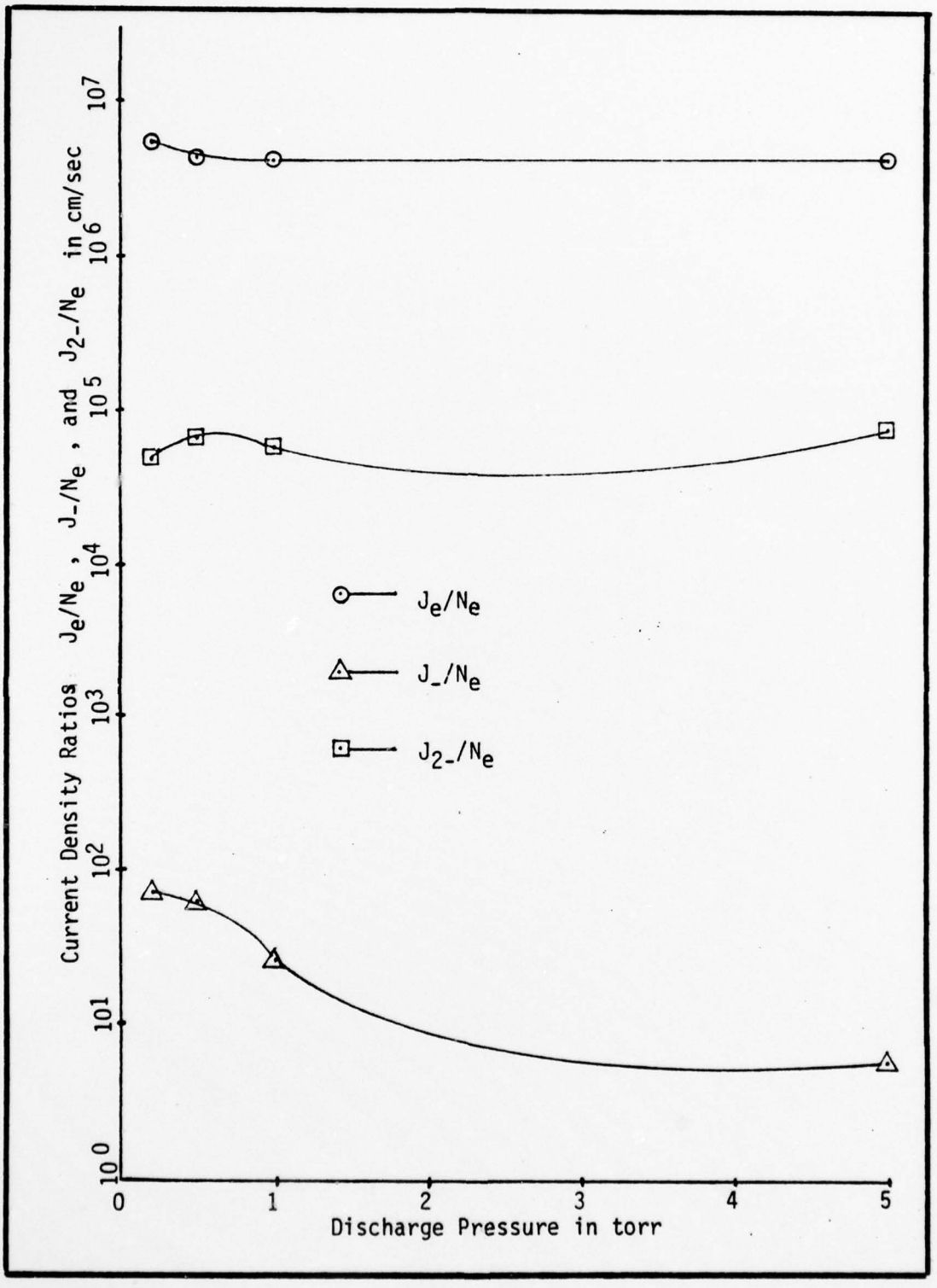

Figure 6-3. Equilibrium Radial Current Density Ratios vs. Pressure for the Four Species, Four Reaction Model

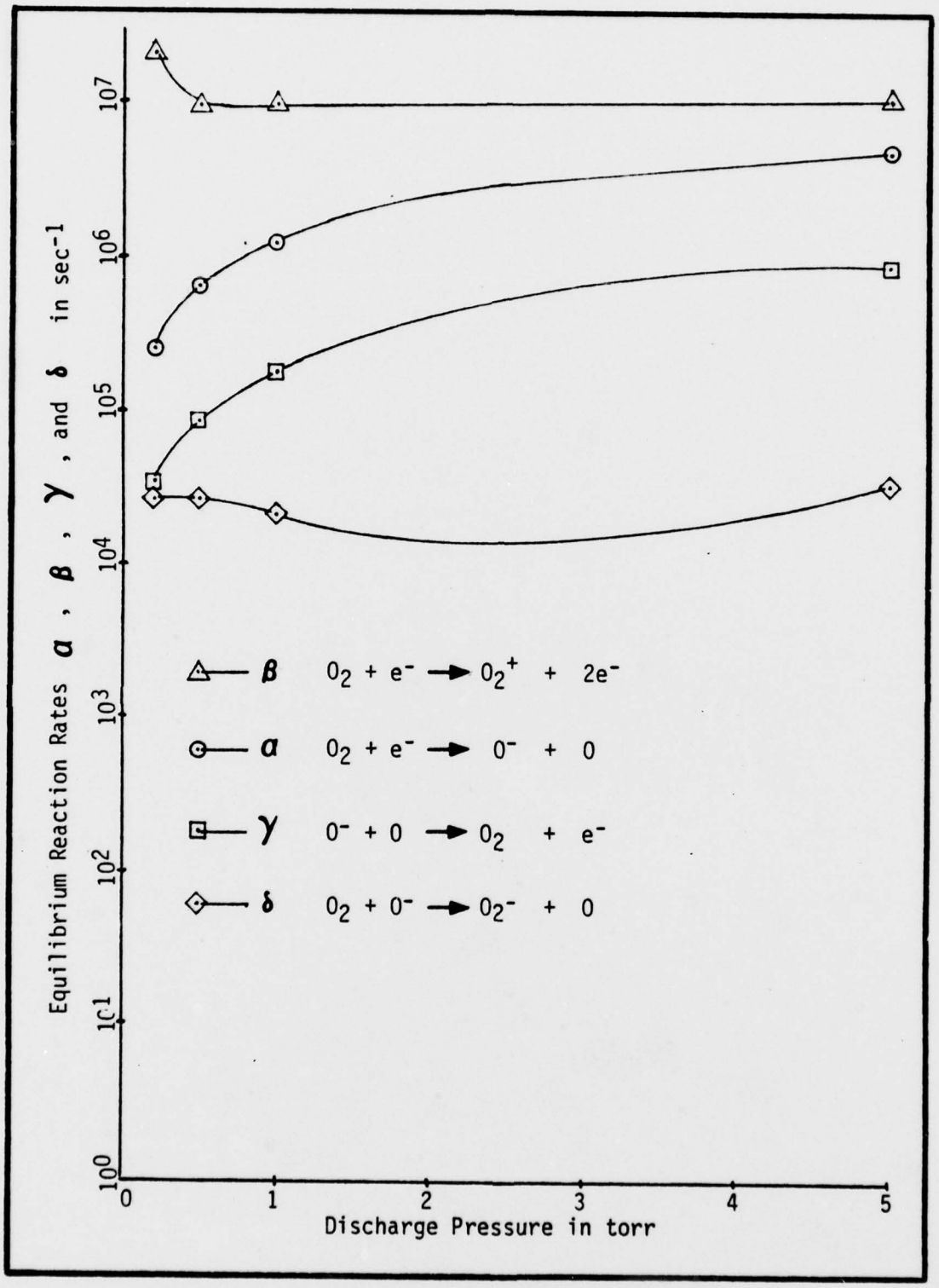

Figure 6-4. Equilibrium Reaction Rates vs. Pressure for the Four Species, Four Reaction Model

VII. Other Models

In order to further test the four species, four reaction model, some other reactions were added. First, the three body attachment reaction

$$O_2 + O_2 + e^- \rightarrow O_2^- + O_2 \qquad (7\text{-}1)$$

was included. It has a reaction rate κ.

Second, the charge transfer reaction

$$O_2^- + O \rightarrow O^- + O_2 \qquad (7\text{-}2)$$

was included along with (7.1).

Four Species, Five Reaction Model

The four species, five reaction oxygen discharge was solved in an identical manner to the four species, four reaction model discussed in Chapter VI. The equations which constitute the characteristic value problem are found in Appendix E and the constants involved in its solution are in Appendix D.

The reaction rate, κ, was taken from Dettmer's dissertation (Ref 2:264). It was represented as

$$\kappa = (1.4\text{x}10^{-29}\text{cm}^6\cdot\text{sec}^{-1})[No_2]^2\ \text{sec}^{-1} \qquad (7.3)$$

In this case, no solutions were achieved. It was possible to find an equilibrium electron temperature, e.g., at 1 torr it was at 3.6 eV. However, at this T_e the number density ratio N_-/N_e held a steady zero value. This was considered unacceptable. Another reaction was therefore added.

Four Species, Six Reaction Model

In an attempt to eat up some of the O_2^- ions which dominated in the four and five reaction models, and in order to rejuvenate the discharge with some O^- ions, the charge transfer reaction (7.2) was added to the system. The equations which define this characteristic value problem are located in Appendix E, and the constants involved are in Appendix D.

The charge transfer reaction rate, ε, was also taken from Dettmer's dissertation (Ref 2:263). The reaction rate was

$$\varepsilon = (3.3\text{x}10^{-10}\text{cm}^3\cdot\text{sec}^{-1})(0.03)[No_2]\ \text{sec}^{-1} \qquad (7.4)$$

This reaction had the desired effect of drastically increasing the population of O^- ions, but it also disastrously reduced the number of O_2^- ions.

The radical in the equation analogous to equation (6.33) began producing complex valued ratios for the number density ratio N_-/N_e in the regions near where the other models' equilibrium T_e's were located.

The present treatment of the four species, six reaction model was therefore considered unphysical using only the reactions postulated.

VIII. Discussion

The objective of this thesis was to obtain reasonable models for the three and four species oxygen discharges that included radial migration of the electrons and ions. Using a three moment model and making appropriate simplifying assumptions, it has been shown that both the three and four species oxygen discharges may be modeled as basic characteristic value problems for the electron temperature. By using a Bessel type substitution, it has been shown that the differential moment equations can be transformed into a simple set of algebraic equations.

The facility with which the models proposed have been solved is due directly to the analytic technique formulated by Lee and elaborated upon in this thesis.

It has not been claimed that the solutions obtained are unique. It is not clear at this time that there are no other solutions. In fact, a judicious combination of Bessel function substitutions is the most obvious method to use for attempting to produce other solutions.

The models analyzed quantitatively here are based on numerous assumptions and approximations. This is undoubtedly not the true situation. Dettmer thinks that the electron distribution is between a Maxwellian and a Druyvesteyn (Ref 2:221). Therefore, it is not suggested that the models displayed here will provide quantitative results for the actual discharge.

One drawback to the technique used to solve the discharge models is that it cannot handle neutral particles. The magic substitution will no longer smoothly transition the system of differential discharge equations into an algebraic set of equations. However, this is not

fatal and may be easily handled if the equilibrium concentration of the neutrals is known.

The mathematical approach demonstrated in this thesis provides a rapid and a convenient way to begin the analysis of gas discharge models. It may provide useful preliminary results in parametric studies which, if carried out with more accurate models, would be much more expensive.

The three species, three reaction model is probably better than the four species model, because it corresponded closer to what has been observed in the actual discharge. Specifically, the O^- ion and not the O_2^- ion is considered to be the dominant species (Ref 3).

The models do provide an analytic tool for beginning to unravel the trends within the discharge. Thus, the mathematical technique upon which the models are based produces solutions which indicate that the radial profiles are Bessel. Also, the models indicate that ions and not electrons are the numerically dominant particles in the discharge at low pressure. The three species model resulted in O^- ions diffusing radially toward the axis of the tube. Sabadil arrived at this same result in his numerical solution to the three species discharge (Ref 17: 235). The fact that the equilibrium electron temperature and the number density ratio, $\frac{N_-}{N_e}$, decrease with increasing pressure is a physical reality (Ref 3). Thus, despite its simplicity this analytic technique has modeled several physical observables.

The fact that the four species model began to apparently diverge from reality is probably a result of using too few of the thirty odd reactions in which O^- and O_2^- participate (Ref 2:263-266). A more

appropriate set of reactions might have enlivened the four species model. Going to a five or six species system is perhaps more reasonable than using what may be an interim four species system.

To this end, the analytic technique which has been used to model the oxygen discharge is perfectly amenable to extension to systems containing more species and more reactions involving them. In fact, there is theoretically no limit to the number of species that could be maintained in a discharge based on this analytic technique.

Therefore, the outstanding conclusion to be drawn is that Lee's magic substitution, (2.57) and (2.58), and straight-forward generalizations of that substitution, provide an extremely simple and powerful tool for analyzing multi-component gas discharges.

IX. Recommendations

Using the analytic technique developed here, the four species model needs to be improved. It may be useful to add reactions in forward and reverse pairs.

Throughout the entire discussion, the Maxwellian electron temperature dependence of $m_e\nu_e$ has been neglected. The models were perfectly amenable to entering the collision frequency, ν_e, as

$$\nu_e \propto \bar{\sigma}_M(T_e)\ T_e^{\frac{1}{2}}\ No_2 \qquad (9.1)$$

Where $\bar{\sigma}_M$ is the average momentum transfer cross section for electrons in oxygen. In order to do this, however, it is necessary to know the average fractional momentum loss per collision. In this same vein, the discharge cannot be completely solved unless the energy collision frequency, ν_{eo}, is known. Neither of these fractional losses were known. Therefore, it is recommended that a careful analysis be done to determine ν_e, and ν_{eo} as functions of the electron temperature T_e in the oxygen discharge.

Because this model has the ability to theoretically handle any number of charged particles or species, an analysis which includes all the species in the oxygen discharge should be systemically attempted.

Finally, it may be possible to combine the effects of gas heating and this plasma model. Such an undertaking would represent a synthesis of the thesis done by Moore and the models contained herein (Ref 14).

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Appendix A

Development of the Moment Equations for a Maxwellian Gas

Moment equations are usually the cornerstone in the development of a plasma discharge model. They are the result of taking successive moments of the Boltzmann transport equation. The treatment followed here draws upon that of Rose and Clark (Ref 16:112-126) and closely parallels that of Lee (Ref 8:1-7).

Each species in a plasma discharge has its own Boltzmann equation. The derivation of the Boltzmann equation is found in most plasma physics textbooks. Here, equations will only be developed for one species, but similar equations may be written for other species in the same discharge. The Boltzmann equation may be written in non-relativistic component form as

$$\frac{\partial f}{\partial t} + v_\ell \frac{\partial f}{\partial x_\ell} + Z \frac{q_o}{m}(E_\ell + \varepsilon_{\ell mn} v_m B_n)\frac{\partial f}{\partial v_\ell} = \left(\frac{\partial f}{\partial t}\right)_{coll} \qquad (A.1)$$

Where f is the distribution function for the species involved and is a function of $\underline{x}$, $\underline{v}$, and t the position of a particle in position space, the velocity of a particle in velocity space, and time, respectively:

$$f = f(\underline{x}, \underline{v}, t) \qquad (A.2)$$

The parameters x_ℓ, v_ℓ, v_m are the ℓth components of position and the ℓth and mth components of velocity. E_ℓ and B_n are the ℓth and nth components of the electric field and magnetic field. $\varepsilon_{\ell mn}$ is the permutation symbol. Z is the electrostatic charge number, e.g., ±1, ±2. q_o is the basic electrostatic charge. The mass of the species

is m. The term on the right hand side of equation (A.1) is the collision term, $(\frac{\partial f}{\partial t})_{coll}$, and is the discontinuous time rate of change of the distribution function due to short range collisions.

It will be assumed that there is no applied $\underline{B}$ field and that the self-electric field is negligible. Equation (A.1) becomes

$$\frac{\partial f}{\partial t} + v_\ell \frac{\partial f}{\partial x_\ell} + z \frac{q_o}{m} E_\ell \frac{\partial f}{\partial v_\ell} = \left(\frac{\partial f}{\partial t}\right)_{coll} \tag{A.3}$$

Particle Conservation Equation

A particle conservation equation results when the zeroth moment of the Boltzmann equation is computed by integrating (A.3) over velocity space:

$$\int_{\underline{v}} \frac{\partial f}{\partial t} d\underline{v} + \int_{\underline{v}} v_\ell \frac{\partial f}{\partial x_\ell} d\underline{v} + \frac{zq_o}{m} \int_{\underline{v}} E_\ell \frac{\partial f}{\partial v_\ell} d\underline{v} = \int_{\underline{v}} \left(\frac{\partial f}{\partial t}\right)_{coll} d\underline{v} \tag{A.4}$$

The number density for the species is defined as

$$n \equiv \int_{\underline{v}} f \, d\underline{v} \tag{A.5}$$

The average velocity of the particle is defined as

$$\underline{q} \equiv \frac{1}{n} \int_{\underline{v}} \underline{v} \, f \, d\underline{v} \tag{A.6}$$

Now it is assumed that the distribution function, f, is piecewise continuous. Then (A.4) may be written as

$$\frac{\partial}{\partial t} \int_{\underline{v}} f \, d\underline{v} + \frac{\partial}{\partial x_\ell} \int_{\underline{v}} v_\ell \, f \, d\underline{v} - \int_{\underline{v}} f \frac{\partial v_\ell}{\partial x_\ell} d\underline{v} + \frac{zq_o}{m} \left[\frac{\partial}{\partial v_\ell} \int_{\underline{v}} E_\ell \, f \, d\underline{v} \right.$$

$$\left. - \int_{\underline{v}} f \frac{\partial E_\ell}{\partial v_\ell} d\underline{v} \right] = \int_{\underline{v}} \left(\frac{\partial f}{\partial t}\right)_{coll} d\underline{v} \tag{A.7}$$

Velocity in velocity space is not a function of position. The electric field, $\underline{E}$, is not a function of velocity. Thus, using (A.5) and (A.6), equation (A.7) reduces to the particle conservation equation:

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x_\ell}(nq_\ell) = \int_{\underline{v}} \left(\frac{\partial f}{\partial t}\right)_{coll} d\underline{v} = Q \qquad (A.8)$$

Momentum Transport Equation

The momentum transport equation is obtained by multiplying equation (A.3) by mv_j and integrating over velocity space:

$$m\int_{\underline{v}} v_j \frac{\partial f}{\partial t}\, d\underline{v} + m\int_{\underline{v}} v_j v_\ell \frac{\partial f}{\partial x_\ell}\, d\underline{v} + Zq_o \int_{\underline{v}} v_j E_\ell \frac{\partial f}{\partial v_\ell}\, d\underline{v}$$

$$= m\int_{\underline{v}} v_j \left(\frac{\partial f}{\partial t}\right)_{coll} d\underline{v} \qquad (A.9)$$

Which becomes

$$\frac{\partial}{\partial t}\int_{\underline{v}} v_j f d\underline{v} - \int_{\underline{v}} \frac{\partial v_j}{\partial t} f d\underline{v} + \frac{\partial}{\partial x_\ell}\int_{\underline{v}} v_j v_\ell f d\underline{v} - \int_{\underline{v}} \frac{\partial v_j}{\partial x_\ell} v_\ell f d\underline{v}$$

$$- \int_{\underline{v}} \frac{\partial v_\ell}{\partial x_\ell} v_j f d\underline{v} + \frac{Zq_o}{m}\int_{\underline{v}} v_j \frac{\partial f}{\partial v_\ell} d\underline{v} = \int_{\underline{v}} v_j \left(\frac{\partial f}{\partial t}\right)_{coll} d\underline{v} \qquad (A.10)$$

Now, using equation (A.6) and the fact that velocity components are independent of position components, (A.10) becomes

$$\frac{\partial}{\partial t}(nq_j)+\frac{\partial}{\partial x_\ell}\int_{\underline{v}} v_j v_\ell f d\underline{v} + \frac{Zq_o}{m}E_\ell \int_{\underline{v}} v_j \frac{\partial f}{\partial v_\ell} d\underline{v} = \int_{\underline{v}} v_j \left(\frac{\partial f}{\partial t}\right)_{coll} d\underline{v} \quad (A.11)$$

Define a new velocity, u_k, which is the random velocity about the mean velocity, q_k. This velocity u_k is called the "peculiar velocity":

$$u_k \equiv v_k - q_k \quad (A.12)$$

The second term on the left of (A.11) becomes

$$\frac{\partial}{\partial x_\ell}\int_{\underline{v}} v_j v_\ell f d\underline{v} + \frac{\partial}{\partial x_\ell}\int_{\underline{v}} (u_j+q_j)(u_\ell+q_\ell) f \, d\underline{v} \quad (A.13)$$

$$\frac{\partial}{\partial x_\ell}\int_{\underline{v}} v_j v_\ell f d\underline{v} = \frac{\partial}{\partial x_\ell}\left[\int_{\underline{v}} u_j u_\ell f d\underline{v} + \int_{\underline{v}} q_\ell u_j f d\underline{v} + \int_{\underline{v}} q_j u_\ell f d\underline{v} + q_j q_\ell \int_{\underline{v}} f \, d\underline{v}\right] \quad (A.14)$$

$$\frac{\partial}{\partial x_\ell}\int_{\underline{v}} v_j v_\ell d\underline{v} = \frac{\partial}{\partial x_\ell}\left[\int_{\underline{v}} u_j u_\ell f d\underline{v} + nq_\ell(q_j-q_j) + n(q_\ell-q_\ell)q_j + nq_j q_\ell\right] \quad (A.15)$$

Therefore,

$$\frac{\partial}{\partial x_\ell}\int_{\underline{v}} v_j v_\ell f d\underline{v} = \frac{\partial}{\partial x_\ell}\left[\int_{\underline{v}} u_j u_\ell f d\underline{v} + nq_j q_\ell\right] \quad (A.16)$$

Now, the kinetic stress tensor appears as

$$\sigma_{j\ell} = \int_{\underline{v}} u_j u_\ell f d\underline{v} = \int_{\underline{v}} u_j u_\ell f(\underline{x}, \underline{u}+\underline{q}, t) d\underline{u} \quad (A.17)$$

Also, the third term on the left side of (A.11) may be written

$$\frac{Zq_o}{m}E_\ell\int_{\underline{v}} v_j\frac{\partial f}{\partial v_\ell}d\underline{v} = \frac{Zq_o}{m}E_\ell\left[\frac{\partial}{\partial v_\ell}\int_{\underline{v}} v_j f d\underline{v} - \int_{\underline{v}}\frac{\partial v_j}{\partial v_\ell}f\ d\underline{v}\right] \tag{A.18}$$

$$\frac{Zq_o}{m}E_\ell\int_{\underline{v}} v_j\frac{\partial f}{\partial v_\ell}\ d\underline{v} = \frac{Zq_o}{m}E_\ell\left[\frac{\partial}{\partial v_\ell}(nq_j) - \delta_{j\ell}\ n\right] \tag{A.19}$$

Both n and q_j are independent of v_ℓ. $\delta_{j\ell}$ is the Kronecker delta function. Equation (A.19) becomes

$$\frac{Zq_o}{m}E_\ell\int_{\underline{v}} v_j\ \frac{\partial f}{\partial v_\ell}\ d\underline{v} = -\ \frac{Zq_o}{m}E_j n \tag{A.20}$$

Now, let the collision term on the right side of equation (A.11) be defined as

$$\int_{\underline{v}} v_j\left(\frac{\partial f}{\partial t}\right)_{coll} d\underline{v} \equiv n\ A_j \tag{A.21}$$

Then using (A.16), (A.17), and (A.21), equation (A.11) may be written as:

$$\frac{\partial}{\partial t}\ (nq_j) + \frac{\partial}{\partial x_\ell}\left[nq_jq_\ell + \sigma_{j\ell}\right] = \frac{nZq_o}{m}E_j + n\ A_j \tag{A.22}$$

By expanding, dividing through by n, and using equation (A.8), equation (A.22) becomes

$$\frac{\partial}{\partial t}\ q_j + q_\ell\ \frac{\partial q_j}{\partial x_\ell} = -\ \frac{1}{n}\ \frac{\partial \sigma_{j\ell}}{\partial x_\ell} + \frac{Zq_o}{m}\ E_j + A_j\ -\ \frac{Q}{n}q_j \tag{A.23}$$

It is assumed that the distribution function, f, is the Maxwellian

$$f(\underline{x},\underline{v},t) = n(\frac{m}{2\pi T})^{3/2} \; e^{\left[-\frac{m}{2T}(\underline{v}-\underline{q})^2\right]} \tag{A.24}$$

T is the Maxwellian temperature expressed in energy units; thus, embedded in T is the Boltzmann constant. The quantities n, T, and $\underline{q}$ are functions of $\underline{x}$ and $\underline{t}$. The kinetic stress tensor may be simplified as follows:

$$\sigma_{ij} = \int_{\underline{v}-\underline{q}} (v_i-q_i)(v_j-q_j) f(\underline{x},\underline{v},t) d(\underline{v}-\underline{q}) \tag{A.25}$$

$$\sigma_{ij} = n(\frac{m}{2\pi T})^{3/2} \int_{\underline{u}} u_i u_j \; e^{-\frac{m}{2T}u^2} \; d\underline{u} \tag{A.26}$$

$$\sigma_{ij} = \langle u_i u_j \rangle \tag{A.27}$$

The quantity $\langle u_i u_j \rangle$ is the average value of the product $u_i u_j$. Assume that u_i and u_j are uncorrelated. Then equation (A.27) becomes

$$\sigma_{ij} = \langle u_i \rangle \langle u_j \rangle \tag{A.28}$$

But the average values of u_i or u_j are just zero. Therefore, the kinetic stress tensor is zero unless i is equal to j. This result is reasonable in light of the fact that a Maxwellian gas will not support a shear; thus, only the diagonal components of the kinetic stress tensor are non-zero. These three components may be evaluated.

In the spherical coordinate system (u, ϕ, θ) the kinetic stress tensor becomes

$$\sigma_{kk} = n\left(\frac{m}{2\pi T}\right)^{3/2} \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} u^4 \cos\theta \sin\theta \; e^{-\frac{m}{2T}u^2} \, du \, d\theta \, d\phi \qquad (A.29)$$

Which, when carried out, is

$$\sigma_{kk} = \frac{nT}{m} \qquad (A.30)$$

Thus, for a Maxwellian gas the kinetic stress tensor is

$$\sigma_{ij} = \frac{nT}{m}\delta_{ij} \qquad (A.31)$$

Then the momentum equation (A.23) becomes

$$\frac{\partial}{\partial t}q_j + q_\ell \frac{\partial}{\partial x_\ell} q_j = -\frac{1}{n}\frac{\partial}{\partial x_j}\left(\frac{nT}{m}\right) + \frac{Zq_o}{m}E_j + A_j - \frac{Q}{n}q_j \qquad (A.32)$$

Energy Conservation Equation

An energy equation results when the second moment of the Boltzmann equation is taken. This is accomplished by multiplying the Boltzmann equation, (A.3), by $\frac{m}{2}v_k v_k$ and then integrating over velocity space:

$$\frac{m}{2}\int_{\underline{v}} v_k v_k \frac{\partial f}{\partial t} d\underline{v} + \frac{m}{2}\int_{\underline{v}} v_k v_k v_\ell \frac{\partial f}{\partial x_\ell} d\underline{v} + \frac{Zq_o}{2}E_\ell \int_{\underline{v}} v_k v_k \frac{\partial f}{\partial v_\ell} d\underline{v}$$

$$= \frac{m}{2}\int_{\underline{v}} v_k v_k \left(\frac{\partial f}{\partial t}\right)_{coll} d\underline{v} \qquad (A.33)$$

Define the quantities

$$nU \equiv \frac{m}{2}\int_{\underline{v}} v_k v_k \; f \; d\underline{v} \tag{A.34}$$

$$n\Theta \equiv \frac{m}{2}\int_{\underline{v}} (v_k - q_k)(v_k - q_k) \; f \; d\underline{v} \tag{A.35}$$

The quantity U is the average kinetic energy per particle. Analogous to the peculiar velocity defined by equation (A.12), the quantity Θ may be considered a "peculiar energy" or random energy. Expanding and simplifying (A.35) the quantity $n\Theta$ may be written

$$n\Theta = nU - \frac{m}{2} q_k q_k \tag{A.36}$$

Also, utilizing equations (A.17) and (A.12) in (A.35), it is seen that

$$n\Theta = \frac{m}{2} \sigma_{kk} \tag{A.37}$$

Expanding the second term of equation (A.33) and using equations (A.12) and (A.17), it is seen that

$$\frac{m}{2}\int_{\underline{v}} v_k v_k v_\ell \frac{\partial f}{\partial x_\ell} d\underline{v} = \frac{m}{2} \frac{\partial}{\partial x_\ell}\left[\int_{\underline{v}} u_k u_k u_\ell \; f \; d\underline{v} + q_\ell \sigma_{kk} + 2q_k \sigma_{k\ell} + n q_k q_k q_\ell\right] \tag{A.38}$$

Now, define the heat flux vector as

$$n\Gamma_\ell \equiv \frac{m}{2}\int_{\underline{v}} u_k u_k u_\ell \; f \; d\underline{v} \tag{A.39}$$

The first term in equation (A.33) may be simplified:

$$\frac{m}{2}\int_{\underline{v}} v_k v_k \frac{\partial f}{\partial t} d\underline{v} = -2nq_\ell \tag{A.40}$$

Now, define

$$nP \equiv \frac{m}{2}\int_{\underline{v}} v_k v_k \left(\frac{\partial f}{\partial t}\right)_{coll} d\underline{v} \tag{A.41}$$

Then by utilizing equations (A.34), (A.38), (A.40), and (A.41) in equations (A.33), it is found that

$$\frac{\partial}{\partial t}(nU) + \frac{\partial}{\partial x_\ell}\left[n\Gamma_\ell + \frac{m}{2}(q_\ell \sigma_{kk} + 2q_k \sigma_{k\ell} + nq_k q_k q_\ell)\right]$$

$$= Zq_o E_\ell n q_\ell + nP \tag{A.42}$$

Now, using equations (A.36) and (A.37), equation (A.42) can be rewritten:

$$\frac{\partial}{\partial t}\left[n\Theta + \frac{m}{2} q_k q_k\right] + \frac{\partial}{\partial x_\ell}\left[n\Gamma_\ell + nq_\ell \Theta + mq_k \sigma_{k\ell} + \frac{mn}{2} q_k q_k q_\ell\right]$$

$$= Zq_o E_\ell n q_\ell + nP \tag{A.43}$$

Expanding this equation and using the particle conservation equation (A.8), equation (A.43) becomes

$$\Theta Q + n\left[\frac{\partial \Theta}{\partial t} + q_\ell \frac{\partial \Theta}{\partial x_\ell}\right] + \frac{\partial}{\partial x_\ell}(n\Gamma_\ell) + nm\left[\frac{1}{2}\frac{\partial}{\partial t}(q_k q_k) + \frac{1}{2} q_\ell \frac{\partial}{\partial x_\ell}(q_k q_k)\right.$$

$$\left. + \frac{q_k}{n}\frac{\partial}{\partial x_\ell}\sigma_{k\ell}\right] = -m\sigma_{k\ell}\frac{\partial}{\partial x_\ell} q_k - \frac{m}{2} q_k q_k Q + Zq_o n q_\ell E_\ell + nP \tag{A.44}$$

The result of contracting the momentum transport equation, (A.23), with q_j is

$$\frac{1}{2}\frac{\partial}{\partial t}(q_j q_j) + \frac{1}{2} q_\ell \frac{\partial}{\partial x_\ell}(q_j q_j) + \frac{q_j}{n}\frac{\partial}{\partial x_\ell}\sigma_{k\ell} = \frac{Zq_o E_j q_j}{m} + A_j q_j - \frac{Q}{n} q_j q_j \tag{A.45}$$

Using the result of (A.45) in (A.44) one finds that

$$\frac{\partial}{\partial t}\Theta + q_\ell \frac{\partial}{\partial x_\ell}\Theta = -\frac{m}{n}\sigma_{k\ell}\frac{\partial}{\partial x_\ell} q_k - \frac{1}{n}\frac{\partial}{\partial x_\ell}(n\Gamma_\ell) - mA_j q_j + P + \frac{Q}{n}\frac{m}{2} q_k q_k - \frac{Q\Theta}{n} \tag{A.46}$$

Equation (A.46) is the energy conservation equation.

Using the Maxwellian distribution results, (A.31), equation (A.37) is

$$\Theta = \frac{m}{2n}\sigma_{kk} = \frac{m}{2n}\left(\frac{3nT}{m}\right) = \frac{3}{2} T \tag{A.47}$$

For the Maxwellian distribution the peculiar velocities are isotropic; thus, equation (A.39) for the heat flux vector may be written

$$\Gamma_\ell = \frac{m}{2n}\int_{\underline{v}} u^3 \, f \, d\underline{v} \tag{A.48}$$

Equation (A.48) is an odd function of u; therefore,

$$\Gamma_\ell = 0 \tag{A.49}$$

Utilizing (A.47) and (A.49) in equation (A.46), the energy conservation equation is

$$\frac{\partial T}{\partial t} + q_\ell \frac{\partial T}{\partial x_\ell} = -\frac{2}{3} T \frac{\partial}{\partial x_\ell} q_\ell - \frac{2}{3} m A_j q_j + \frac{2}{3} P + \frac{Q}{n}\frac{m}{3} q_k q_k - \frac{Q}{n} T \tag{A.50}$$

Summary

The zeroth, first, and second moments of the Boltzmann transport equation yield respectively, a particle conservation equation, a momentum conservation equation, and an energy conservation equation. If it is assumed that there is no applied $\underline{B}$ field, that the self electric field is negligible, and that the distribution function for the species is Maxwellian, then the following three moment equations result:

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x_\ell}(nq_\ell) = Q \tag{A.8}$$

$$\frac{\partial}{\partial t}q_j + q_\ell \frac{\partial}{\partial x_\ell}q_j = -\frac{1}{n}\frac{\partial}{\partial x_j}\left(\frac{nT}{m}\right) + \frac{Zq_o E_j}{m} + A_j - \frac{Q}{n}q_j \tag{A.21}$$

$$\frac{\partial T}{\partial t} + q_\ell \frac{\partial T}{\partial x_\ell} = -\frac{2}{3}T\frac{\partial}{\partial x_\ell}q_\ell - \frac{2}{3}mA_j q_j + \frac{2}{3}P + \frac{Q}{n}\frac{m}{3}q_k q_k - \frac{Q}{n}T \tag{A.50}$$

For a gas containing more than one species, these equations must be written for each species. For one species the production term was represented as Q; however, for a multi-species system, each species would have a different production term. Such a system of equations is related through their production terms.

Appendix B

Equilibrium Equations for a Two Species Gas Discharge

Equilibrium equations for a two species gas discharge, consisting of electrons, singly charged positive ions, and a neutral background gas, are developed here. The system will be assumed to have cylindrical symmetry as shown in Figure B-1.

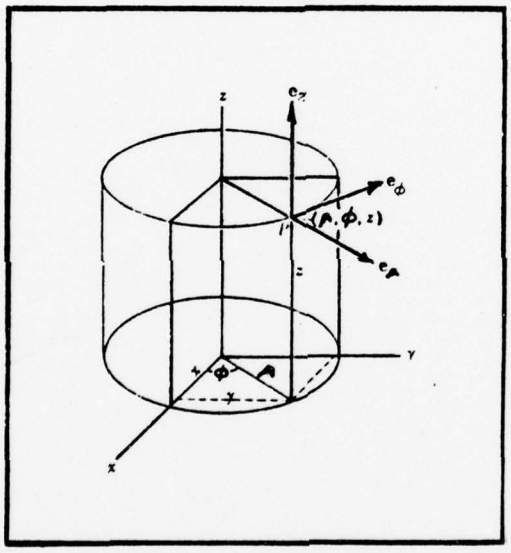

Figure B-1. Cylindrical System (Ref 19:138)

It will be assumed that the system is in equilibrium. It will also be assumed that the average velocity, $\underline{q}$, has only radial and axial components, which are functions of the distance r from the axis:

$$\underline{q} = [v(r), o, u(r)] \qquad (B.1)$$

It is assumed that the electric field $\underline{E}$ has only radial and axial components. The radial component is a function of r, but the axial

component is a constant:

$$\underline{E} = [E_r(r),\ 0,\ E_o] \tag{B.2}$$

Particle Conservation Equations

For a two component system in equilibrium, there will be two particle conservation equations. Using equation (A.8), the electron conservation equation becomes

$$\frac{\partial}{\partial x_\ell}(n_e q_\ell) = \nabla\cdot(n_e \underline{q}) = \frac{1}{r}\frac{\partial}{\partial r}(r n_e v_e) = Q_e \tag{B.3}$$

Which is

$$n_e v_e' + v_e n_e' + \frac{n_e v_e}{r} = Q_e \tag{B.4}$$

The quantity, Q_e, is the production term for electrons. The quantity n_e is the number density for electrons. v_e is the radial component of the average velocity, and the prime indicates differentiation with respect to the radial distance r. A similar equation may be written for ions:

$$n_i v_i' + v_i n_i' + \frac{n_i v_i}{r} = Q_i \tag{B.5}$$

Momentum Conservation Equations

In equilibrium the momentum conservation equation (A.32) is

$$q_\ell \frac{\partial}{\partial x_\ell} q_j = -\frac{1}{n_e m_e}\frac{\partial}{\partial x_j}(n_e T_e) + \frac{Zq_o}{m_e}E_j + A_j - \frac{Q_e}{n_e}q_j \tag{B.6}$$

T_e is the Maxwellian electron temperature, and m_e is the mass of the electron. The term on the left may be written as (Ref 11)

$$q_\ell \frac{\partial}{\partial x_\ell} q_j = (\underline{q}\cdot\nabla)\underline{q} = \nabla(\tfrac{1}{2}\,\underline{q}\cdot\underline{q}) - \underline{q} \times \nabla \times \underline{q} \qquad \text{(B.7)}$$

Now, for the system postulated

$$\nabla(\tfrac{1}{2}\, q\cdot q) = \hat{e}_r v_e \frac{\partial v_e}{\partial r} + \hat{e}_r u_e \frac{\partial u_e}{\partial r} \qquad \text{(B.8)}$$

And

$$\nabla x \underline{q} = \frac{1}{r} \begin{vmatrix} \hat{e}_r & \hat{r}e_\phi & \hat{e}_z \\ \frac{\partial}{\partial r} & \frac{\partial}{\partial \phi} & \frac{\partial}{\partial z} \\ v_e & 0 & u_e \end{vmatrix} = -\hat{e}_\phi \frac{\partial u_e}{\partial r} \qquad \text{(B.9)}$$

Therefore,

$$-\underline{q}x(\nabla x \underline{q}) = - \begin{vmatrix} \hat{e}_r & \hat{e}_\phi & \hat{e}_z \\ v_e & 0 & u_e \\ 0 & -\frac{\partial u_e}{\partial r} & 0 \end{vmatrix} = \hat{e}_z v_e \frac{\partial u_e}{\partial r} - \hat{e}_r u_e \frac{\partial u_e}{\partial r} \qquad \text{(B.10)}$$

Then,

$$q_\ell \frac{\partial}{\partial x_\ell} q_j = \hat{e}_r v_e v_e' + \hat{e}\, v_e u_e' \qquad \text{(B.11)}$$

The first term on the right of equation (B.6) can be written as two component equations. The radial component is the only one which survives in the discharge, since it is assumed that n_e and T_e are functions of r only:

$$- \frac{1}{n_e m_e} \frac{\partial}{\partial x_j}(n_e T_e) = - \frac{\hat{e}_r}{n_e m_e}(n_e T_e) \qquad (B.12)$$

The second term on the right of equation (B.6) generates the two components

$$\hat{e}_r \frac{z\, q_o\, E_r}{m_e} \quad ; \quad \hat{e}_z \frac{z\, q_o\, E_o}{m_e} \qquad (B.13)$$

The collision term in the momentum equation is A_j and is defined by equation (A.21). Lee models this term for electrons (Ref 8:8) as

$$A_j^{(e)} = -\nu_e\left(q_j^{(e)} - q_j^{(o)}\right) . \qquad (B.14)$$

A similar equation may be written for the ions:

$$A_j^{(i)} = -\nu_i\left(q_j^{(i)} - q_j^{(o)}\right) \qquad (B.15)$$

The superscripts, (e), (i), and (o) represent electrons, ions, and neutral particles, respectively. ν_e is the collision frequency of electrons with neutrals multiplied by the fractional momentum loss that an electron suffers each time it collides with a neutral particle. The fractional momentum loss is the sum of the elastic and inelastic momentum losses. Analogous to ν_e, the term ν_i is the collision frequency of the ions with neutrals multiplied by the fractional momentum loss suffered by an ion in a collision with a neutral. The radial electron and ion terms are

$$A_r^{(e)} = -\nu_e(v_e - v_o) \qquad (B.16)$$

and

$$A_r^{(i)} = -\nu_i(v_i - v_o) \tag{B.17}$$

It will be assumed that the neutral background gas has a negligible radial velocity component v_o. This situation could be achieved by flowing the neutral gas through the discharge tube at a proper speed dependent on the radial velocity of the ions. Thus, equations (B.16) and (B.17) become

$$A_r^{(e)} = -\nu_e v_e \tag{B.18}$$

$$A_r^{(i)} = -\nu_i v_i \tag{B.19}$$

The axial electron and ion collision terms are

$$A_z^{(e)} = -\nu_e(u_e - u_o) \tag{B.20}$$

$$A_z^{(i)} = -\nu_i(u_i - u_o) \tag{B.21}$$

The last term in equation (B.6) is $-\frac{Q}{n}q_j$. This term will be assumed to be negligible. This assumption means that newly born particles have negligible momentum.

Using the results (B.11), (B.12), (B.13), and (B.16) in the equilibrium momentum conservation equation (B.6), the radial momentum conservation equations for the electrons and ions become

$$v_e v_e' = -\frac{1}{n_e m_e}(T_e n_e)' - \frac{q_o E_r}{m_e} - \nu_e v_e \tag{B.22}$$

$$v_i v_i' + -\frac{1}{n_i m_i}(T_i n_i)' + \frac{Zq_o}{m_i}E_r - \nu_i v_i \tag{B.23}$$

Likewise, the axial momentum conservation equations for the electrons and ions become

$$v_e u_e' = - \frac{q_o E_o}{m_e} - \nu_e (u_e - u_o) \tag{B.24}$$

$$v_i u_i' = \frac{Zq_o E_o}{m_i} - \nu_i (u_i - u_o) \tag{B.25}$$

Energy Conservation Equations

At equilibrium the energy conservation equation for electrons, (A.50), is

$$q_\ell \frac{\partial T_e}{\partial x_\ell} = - \frac{2}{3} T_e \frac{\partial q_\ell}{\partial x_\ell} - \frac{2}{3} m_e A_j q_j + \frac{2}{3} P + \frac{Q_e}{n_e} \frac{m_e}{3} q_k q_k - \frac{Q_e T_e}{n_e} \tag{B.26}$$

Since T_e is assumed to be only a function of r, the first term is

$$q_\ell \frac{\partial T_e}{\partial x_\ell} = v_e T_e' \tag{B.27}$$

Also,

$$- \frac{2}{3} T_e \frac{\partial q_\ell}{\partial x_\ell} = - \frac{2}{3} T_e \nabla \cdot \underline{q} = - \frac{2}{3} T_e \left[\frac{1}{r} \frac{\partial}{\partial r} (r v_e) \right] = - \frac{2}{3} T_e \left(v_e' + \frac{v_e}{r} \right) \tag{B.28}$$

Using (B.18) and (B.20), the third term in equation (B.26) becomes

$$- \frac{2}{3} m_e A_j q_j = - \frac{2}{3} m_e \underline{A} \cdot \underline{q} = \frac{2}{3} m_e \nu_e (v_e^2 + u_e^2 - u_e u_o) \tag{B.29}$$

Since u_o was assumed to be negligible, certainly

$$(v_e^2 + u_e^2) \gg u_e u_o \tag{B.30}$$

Therefore,

$$-\frac{2}{3}m_e A_j q_j = \frac{2}{3}m_e \nu_e (v_e^2 + u_e^2) \tag{B.31}$$

The collision term P for electrons will be treated in a manner similar to Lee's treatment (Ref 7:8) and modeled as

$$P^{(e)} = -\nu_{eo}(T_e - T_o) \tag{B.32}$$

The quantity ν_{eo} is the collision frequency of electrons with neutrals multiplied by the fractional energy loss suffered by the electrons per collision. Also, it may be assumed that the Maxwellian electron temperature T_e is much greater than that of the background gas T_o. Therefore, the electron collision term is

$$P^{(e)} = -\nu_{eo} T_e \tag{B.33}$$

Likewise, the collision term for the ions may be written

$$P^{(i)} = -\nu_{io}(T_i - T_o) \tag{B.34}$$

Again, ν_{io} is the collision frequency of ions colliding with neutrals multiplied by the fractional energy loss suffered by the ions per collision.

The last two terms of equation (B.26) may be written as

$$\frac{Q_e}{n_e}\left[\frac{m_e}{3}q_k q_k - T_e\right] \tag{B.35}$$

This term will be assumed to be zero, because it represents the approximate difference between the kinetic and thermal energy of newly born particles. This difference is assumed to be negligibly small. The same

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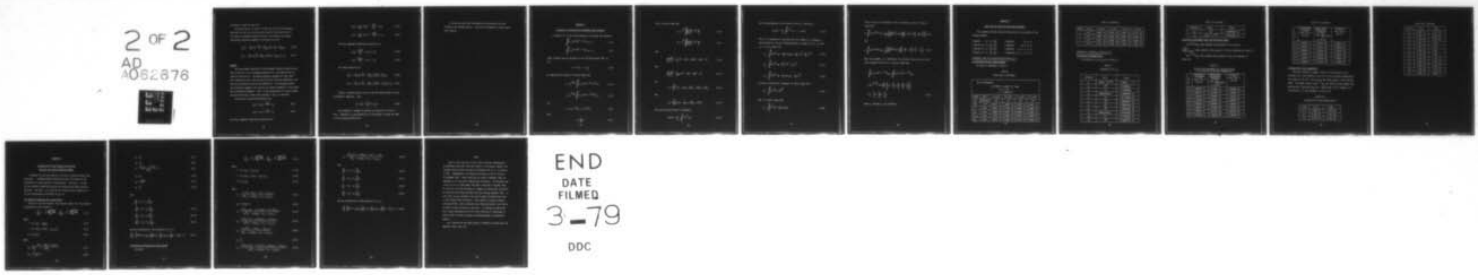

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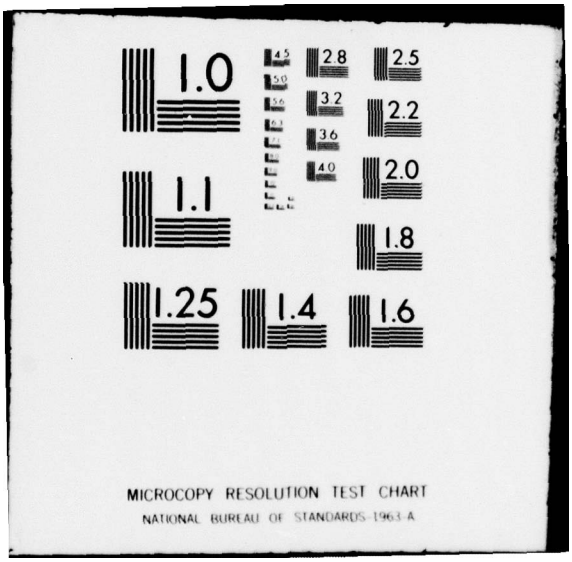
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assumption is made for the ions.

Using the results of (B.27), (B.28), and (B.31) with analogous equations for the ions, and using the results (B.33) and (B.34) in the energy conservation equation (B.26), the following two energy conservation equations emerge for electrons and ions:

$$v_e T_e' = -\frac{2}{3}T_e\left(v_e' + \frac{v_e}{r}\right) + \frac{2}{3}m_e\nu_e\left(v_e^2 + u_e^2\right) - \frac{2}{3}\nu_{eo}T_e \qquad \text{(B.36)}$$

$$v_i T_i' = -\frac{2}{3}T_i\left(v_i' + \frac{v_i}{r}\right) + \frac{2}{3}m_i\nu_i\left(v_i^2 + u_i^2\right) - \frac{2}{3}\nu_{io}\left(T_i - T_o\right) \qquad \text{(B.37)}$$

Summary

The three moment equations of the Boltzmann transport equation were used to derive a set of discharge equations for a two species gas discharge at equilibrium. The moment equations assumed only that there was no applied $\underline{B}$ field, that the self-electric field was negligible, and that the distribution function was Maxwellian. The discharge system had cylindrical symmetry, but none of the vector parameters in the system had an azimuthal component. Also, it was assumed that all scalar parameters were functions of the radial distance r only, or constants.

The particle conservation equations are

$$n_e v_e' + v_e n_e' + \frac{n_e v_e}{r} = Q_e \qquad \text{(B.4)}$$

$$n_i v_i' + v_i n_i' + \frac{n_i v_i}{i} = Q_i \qquad \text{(B.5)}$$

The radial momentum conservation equations are

$$v_e v_e' = \frac{-1}{n_e m_e} (T_e n_e)' - \frac{q_o E_r}{m_e} - \nu_e v_e \qquad (B.22)$$

$$v_i v_i' = \frac{-1}{n_i m_i} (T_i n_i)' + \frac{Zq_o E_r}{m_i} - \nu_i v_i \qquad (B.23)$$

The axial momentum conservation equations are

$$v_e u_e' = \frac{-q_o E_o}{m_e} - \nu_e (u_e - u_o) \qquad (B.24)$$

$$v_i u_i' = \frac{Zq_o E_o}{m_i} - \nu_i (u_i - u_o) \qquad (B.25)$$

The energy equations are

$$v_e T_e' = -\frac{2}{3} T_e \left(v_e' + \frac{v_e}{r}\right) + \frac{2}{3} m_e \nu_e (v_e^2 + u_e^2) - \frac{2}{3} \nu_{eo} T_e \qquad (B.36)$$

$$v_i T_i' = -\frac{2}{3} T_i \left(v_i' + \frac{v_i}{r}\right) + \frac{2}{3} m_i \nu_i (v_i^2 + u_i^2) - \frac{2}{3} \nu_{io} (T_i - T_o) \qquad (B.37)$$

Poisson's equation may be used to close the above system of eight differential equations. Thus,

$$E_r' + \frac{1}{r} E_r = \frac{q_o}{\varepsilon_o} (Z n_i - n_e) \qquad (B.38)$$

The discharge is assumed to operate at pressures of 5 torr or less. Therefore, ε_o the permittivity of free space is almost the same as the discharge permittivity.

It should be noted that the equations derived herein are not limited to two charged species. They may be extended to include other ionic species.

Appendix C

Evaluation of Dissociative Attachment Rate Integrals

In Chapter III it was found necessary to evaluate the integrals

$$\int_0^\infty x^4 \, e^{-(0.19x^2 + x/T_e)} \, dx = F \tag{C.1}$$

$$\int_0^\infty x^3 \, e^{-(0.19x^2 + x/T_e)} \, dx = G \tag{C.2}$$

These integrals may be evaluated in the following manner (Ref 11).

Let

$$a = 0.19 \; ; \quad b = \frac{1}{T_e} \tag{C.3}$$

By completing the square, it may be shown that

$$F = e^{b^2/4a} \int_0^\infty x^4 \, e^{-(\sqrt{a}x + b/2\sqrt{a})^2} \, dx \tag{C.4}$$

$$G = e^{b^2/4a} \int_0^\infty x^3 \, e^{-(\sqrt{a}x + b/2\sqrt{a})^2} \, dx \tag{C.5}$$

Let

$$w = \sqrt{a} + b/2\sqrt{a} \; ; \; g = b/2\sqrt{a} \tag{C.6}$$

Then

$$x = \frac{w-g}{\sqrt{a}} \tag{C.7}$$

Then it may be shown that

$$F_T = e^{g^2} \int_g^\infty \left(\frac{w-g}{\sqrt{a}}\right)^4 e^{-w^2} \frac{dw}{\sqrt{a}} \tag{C.8}$$

$$G_T = e^{g^2} \int_g^\infty \left(\frac{w-g}{\sqrt{a}}\right)^3 e^{-w^2} \frac{dw}{\sqrt{a}} \tag{C.9}$$

Now

$$\left(\frac{w-g}{\sqrt{a}}\right)^4 = \frac{1}{a^2} (w^4 - 4w^3g + 6w^2g^2 - 4wg^3 + g^4) \tag{C.10}$$

And

$$\left(\frac{w-g}{\sqrt{a}}\right)^3 = \frac{1}{a^{3/2}} (w^3 - 3w^2g + 3wg^2 - g^3) \tag{C.11}$$

Let

$$F_T = \frac{e^{g^2}}{a^2} (F_1 - 4gF_2 + 6g^2F_3 - 4g^3F_4 + g^4F_5) \tag{C.12}$$

And

$$G_T = \frac{e^{g^2}}{a^{3/2}} (F_2 - 3gF_3 + 3g^2F_4 - g^3F_5) \tag{C.13}$$

The error function erf(k) is defined as

$$\text{erf}(k) = \frac{2}{\sqrt{\pi}} \int_0^k e^{-s^2} ds \tag{C.14}$$

And the complementary error function erfc(k) is defined as

$$\operatorname{erfc}(k) = \frac{2}{\sqrt{\pi}} \int_k^\infty e^{-s^2}\, ds = 1 - \operatorname{erf}(k) \tag{C.15}$$

Thus, it is necessary to evaluate the five integrals F_1 through F_5. Using Leibnitz's rule for differentiating an integral for F_1, F_2, and F_3, it may be shown that

$$F_1 = \int_g^\infty w^4 e^{-w^2}\, dw = \frac{3\sqrt{\pi}}{8} \operatorname{erfc}(g) + \frac{3g}{4} e^{-g^2} + \frac{g^3}{2} e^{-g^2} \tag{C.16}$$

$$F_2 = \int_g^\infty w^3 e^{-w^2}\, dw = \frac{g^2}{2} e^{-g^2} + \frac{1}{2} e^{-g^2} \tag{C.17}$$

$$F_3 = \int_g^\infty w^2 e^{-w^2}\, dw = \frac{\sqrt{\pi}}{4} \operatorname{erfc}(g) + \frac{g}{2} e^{-g^2} \tag{C.18}$$

By using a differential integrand, it may be shown that

$$F_4 = \int_g^\infty w e^{-w^2} dw = \frac{e^{-g^2}}{2} \tag{C.19}$$

And it is easily shown that

$$F_5 = \int_g^\infty e^{-w^2}\, dw = \frac{\sqrt{\pi}}{2} \operatorname{erfc}(g) \tag{C.20}$$

Now by using (C.16) through (C.20) to evaluate F_T and G_T it may be shown that

$$F = \int_0^\infty x^4 e^{-(ax^2+bx)} dx = \frac{1}{a^{5/2}} \left\{ \left[\frac{\sqrt{\pi}}{2} e^{g^2} \operatorname{erfc}(g) \right] \left[\frac{3}{4} + 3g^2 + g^4 \right] - \frac{5}{4}g - \frac{g^3}{2} \right\} \quad (C.21)$$

And

$$G = \int_0^\infty x^3 e^{-(ax^2+bx)} dx = \frac{1}{a^2} \left\{ \left[\frac{\sqrt{\pi}}{2} e^{g^2} \operatorname{erfc}(g) \right] \left[-\frac{3g}{2} - g^3 \right] + \frac{g^2}{2} + \frac{1}{2} \right\} \quad (C.22)$$

When the parameter g is returned to its original form using (C.6) and then evaluated using (C.3), it may be shown that

$$\int_0^\infty x^4 e^{-(0.19x^2 + x/T_e)} dx + \int_0^\infty x^3 e^{-(0.19x^2 + x/T_e)} dx$$

$$= \frac{\sqrt{\pi}}{2} e^{d_1/T_e^2} \operatorname{erfc}\left(\frac{d_2}{T_e}\right) \left[d_3 - \frac{d_4}{T_e} + \frac{d_5}{T_e^2} - \frac{d_6}{T_e^3} + \frac{d_7}{T_e^4} \right]$$

$$+ d_8 - \frac{d_9}{T_e} + \frac{d_{10}}{T_e^2} - \frac{d_{11}}{T_e^3} \quad (C.23)$$

Where d_1 through d_{11} are constants.

Appendix D

Data from the Three and Four Species Models

This appendix contains numerical data used in the solution of the following models:

3 Species	(e^-, O^-, O_2^+);	3 Reaction	(α, β, γ)
4 Species	(e^-, O^-, O_2^+, O_2^-);	4 Reaction	$(\alpha, \beta, \gamma, \delta)$
4 Species	(e^-, O^-, O_2^+, O_2^-);	5 Reaction	$(\alpha, \beta, \gamma, \delta, \kappa)$
4 Species	(e^-, O^-, O_2^+, O_2^-);	6 Reaction	$(\alpha, \beta, \gamma, \delta, \kappa, \varepsilon)$

Parameters Used for Evaluating Equilibrium T_e's in the Three and Four Species Models

All data is tabulated in Table V.

Table V

Data Used in the Models

For all pressures:

T_o @ 300°K = 4.14132 -14 ergs

R = 1.1 cm

σ_i = 2.1862 cm^{-1}

Symbol	Units	0.2 torr	0.5 torr	1.0 torr	5.0 torr
E/p	V/cm·torr	40	30	20	10
NO_2	cm^{-3}	6.4371 15	1.6093 16	3.2185 16	1.6093 17
$m_-\nu_-$	g/sec	7.9307 -17	2.1796 -16	4.8693 -16	2.9989 -15
$m_+\nu_+$	g/sec	1.8825 -16	4.6031 -16	8.8508 -16	4.2842 -15
$m_{2-}\nu_{2-}$	g/sec	1.7780 -16	4.5641 -16	9.4793 -16	4.4428 -15
$m_e\nu_e$	g/sec	3.6575 -18	3.3168 -18	2.9127 -18	2.0025 -18

Table V--continued

Symbol	Units	0.2 torr	0.5 torr	1.0 torr	5.0 torr
γ	sec^{-1}	3.6691 04	9.1730 04	1.8345 05	9.1730 05
δ	sec^{-1}	2.8967 04	2.8967 04	2.2529 04	4.0233 05
κ	sec^{-1}	5.8011 02	3.6258 03	1.4502 04	3.6258 05
ε	sec^{-1}	6.3727 04	1.5932 05	3.1863 05	1.5932 06

Constants c_1 through c_{13} Used for the Dissociative Attachment Rate

The values of c_1 to c_{13} are in Table VI.

Table VI

Constants c_1 to c_{13}

Constants	Units	Value
c_1	$cm^3 sec^{-1} eV^{-7/2}$	1.840411 -11
c_2	eV^2	1.315789473
c_3	eV	1.147078669
c_4	dimensionless	4.766254858 01
c_5	eV	1.811176846 02
c_6	eV^2	2.508555187 02
c_7	eV^3	1.588751618 02
c_8	eV^4	1.100243502 02
c_9	dimensionless	5.263157895 01
c_{10}	eV	9.112115462 01
c_{11}	eV^2	6.925207753 01

Table VI--continued

Constants	Units	Value
c_{12}	eV^3	4.795850240 01
c_{13}	$cm^3 sec^{-1} eV^{-5/2}$	4.196137080 -10

Dissociative Attachment Rates and Ionization Rates

The $^{\alpha(T_e)}/_{No_2}$ rates computed using equation (3.13) and the $[\frac{\alpha(T_e)}{No_2}]_{approx}$ rates computed using equation (3.16) are tabulated in Table VII.

The $^{\beta(T_e)}/_{No_2}$ rates computed using equation (4.8) are tabulated in Table VII.

Table VII

Dissociative Attachment and Ionization Rates as a Function of Electron Temperature

T_e in eV	Dissociative Attachment Rate $^{\alpha}/_{No_2}$ in cm^3/sec	Approximate Dissociative Attachment Rate $[\frac{\alpha}{No_2}]_{approx}$ in cm^3/sec	Ionization Rate $^{\beta}/_{No_2}$ in cm^3/sec
0.5	2.683649 -14	3.712245 -14	6.525468 -20
1.0	2.687377 -12	9.387083 -12	1.767009 -14
1.5	1.134319 -11	9.180474 -11	1.328730 -12
2.0	2.131484 -11	3.550301 -10	1.258270 -11
2.5	2.923942 -11	9.069265 -10	5.151058 -11
3.0	3.452978 -11	1.843090 -09	1.379607 -10
3.5	3.762679 -11	3.247133 -09	2.891278 -10
4.0	3.913160 -11	5.193019 -09	5.189148 -10

Table VII--continued

T_e in eV	Dissociative Attachment Rate α/No_2 in cm^3/sec	Approximate Dissociative Attachment Rate $[\frac{\alpha}{No_2}]_{approx}$ in cm^3/sec	Ionization Rate β/No_2 in cm^3/sec
4.5	3.954934 -11	7.747175 -09	8.389674 -10
5.0	3.925133 -11	1.097011 -08	1.259933 -09
5.5	3.849647 -11	1.491758 -08	1.792519 -09
6.0	3.746108 -11	1.964150 -08	2.448331 -09
6.5	3.626376 -11	2.519056 -08	3.240551 -09
7.0	3.498369 -11	3.161076 -08	4.184566 -09

Characteristic Value Computation

Table VIII contains a sample listing of the solutions to the characteristic value equation (2.75) for a run of electron temperatures. This sample is for the 1 torr case of the three species, three reaction model. The number density ratio, N_-/N_e, was used to assess whether the equilibrium T_e found was physical. Notice that in this example, the equilibrium T_e is found between 1.4 and 1.6 eV.

Table VIII

Characteristic Value Determination

T_e (eV)	$F(T_e)$	N_-/N_e
0.2	-1.260 -07	-1.707 -02
0.4	-2.478 -07	-3.343 -02
0.6	-3.735 -07	-3.343 -02

Table VIII--continued

T_e (eV)	F (T_e)	N_-/N_e
0.8	-5.558 -07	8.173 -02
1.0	-8.585 -07	3.897 -01
1.2	-1.439 -06	9.278 -01
1.4	-7.772 -07	1.736
1.6	1.561 -06	2.937
1.8	7.902 -06	4.765
2.0	2.100 -05	7.547
2.2	4.454 -05	1.167 01
2.4	8.355 -05	1.753 01
2.6	1.452 -04	2.555 01
2.8	2.399 -04	3.611 01
3.0	3.820 -04	4.958 01

Appendix E

Characteristic Value Systems for the Four Species, Five and Six Reaction Models

In Chapter VII the four species, five and six reaction models were discussed. Although neither system was solved, the setup for the characteristic value problem is included here. The rate, κ, is good for any reaction producing an O_2^- and not affecting the other previous reactions. The rate, ε, is good for any reaction which produces an O^- ion and simultaneously anihilates an O_2^- ion.

Five Reaction Characteristic Value System

Similar to the four species, four reaction model, the five reaction characteristic value system is

$$\left(\frac{N_-}{N_e}\right)_- = \frac{-L-\sqrt{L^2-4KM}}{2K} \; ; \quad \left(\frac{N_-}{N_e}\right)_+ = \frac{-L+\sqrt{L^2-4KM}}{2K} \tag{E.1}$$

Where,

$$K = m_-\nu_-S_1S_3 - m_{2-}\nu_{2-}S_4 \tag{E.2}$$

$$L = m_-\nu_-(R_1S_3 + R_3S_1) - m_{2-}\nu_{2-}R_4 \tag{E.3}$$

$$M = m_-\nu_-R_1R_3 \tag{E.4}$$

Where

$$R_1 = \frac{-T_e}{2T_o} + \frac{\alpha m_-\nu_- + \beta m_+\nu_+ + \kappa m_{2-}\nu_{2-}}{2\sigma_1^2 T_o} \tag{E.5}$$

$$R_2 = \frac{\beta - \alpha - \kappa}{\sigma_1} \tag{E.6}$$

$$R_3 = \frac{\alpha}{\sigma_1} \tag{E.7}$$

$$R_4 = \frac{\kappa}{\sigma_1} \tag{E.8}$$

$$S_1 = \frac{\delta m_{2-} \nu_{2-} - (\gamma+\delta) m_- \nu_-}{2\sigma_1^2 T_o} - 1 \tag{E.9}$$

$$S_2 = \frac{\gamma}{\sigma_1} \tag{E.10}$$

$$S_3 = \frac{-(\gamma+\delta)}{\sigma_1} \tag{E.11}$$

$$S_4 = \frac{\delta}{\sigma_1} \tag{E.12}$$

Now,

$$\frac{N_{2-}}{N_e} = R_1 + S_1 \left(\frac{N_-}{N_e}\right)_{\pm}$$

$$\left(\frac{J_e}{N_e}\right) = R_2 + S_2 \left(\frac{N_-}{N_e}\right)_{\pm} \tag{E.14}$$

$$\left(\frac{J_-}{N_e}\right) = R_3 + S_3 \left(\frac{N_-}{N_e}\right)_{\pm} \tag{E.15}$$

$$\left(\frac{J_{2-}}{N_e}\right) = R_4 + S_4 \left(\frac{N_-}{N_e}\right)_{\pm} \tag{E.16}$$

And the characteristic value equation for T_e is

$$\left(\frac{N_-}{N_e} + \frac{N_{2-}}{N_e}\right)\left[-\sigma_1 T_e + m_e \nu_e \left(\frac{T_e}{N_e}\right)\right] - m_- \nu_- \left(\frac{J_-}{N_e}\right) - m_{2-} \nu_{2-} \left(\frac{J_{2-}}{N_e}\right) = F(T_e) = 0 \tag{E.17}$$

Six Reaction Characteristic Value System

As before,

$$\left(\frac{N_-}{N_e}\right)_- = \frac{-L - \sqrt{L^2-4KM}}{2K} \; ; \quad \left(\frac{N_-}{N_e}\right)_+ = \frac{-L + \sqrt{L^2-4KM}}{2K} \tag{E.18}$$

Where

$$K = m_-\nu_-S_1S_3 - m_{2-}\nu_{2-}S_4 \tag{E.19}$$

$$L = m_-\nu_1(R_1S_3 + S_1R_3) - m_{2-}\nu_{2-}R_4 \tag{E.20}$$

$$M = m_-\nu_-R_1R_3 \tag{E.21}$$

Where

$$R_1 = \frac{\sigma_i(-\sigma_i^2T_e + \beta m_+\nu_+ + \alpha m_-\nu_- + \kappa m_{2-}\nu_{2-})}{2\sigma_i^3T_o - \sigma_i\varepsilon(2m_+\nu_+ + m_-\nu_- + m_{2-}\nu_{2-})} \tag{E.22}$$

$$R_2 = \frac{\beta - \alpha - \kappa}{\sigma_i} \tag{E.23}$$

$$R_3 = \frac{\sigma_i^2(2T_o\alpha - T_e\varepsilon) - \varepsilon(2\alpha-\beta)m_+\nu_+ + \varepsilon(\kappa-\alpha)m_{2-}\nu_{2-}}{2\sigma_i^3T_o - \sigma_i\varepsilon(2m_+\nu_+ + m_-\nu_- + m_{2-}\nu_{2-})} \tag{E.24}$$

$$R_4 = \frac{\sigma_i^2(2T_o\kappa - T_e\varepsilon) + \varepsilon(\beta-2\kappa)m_+\nu_+ + \varepsilon(\alpha-\kappa)m_-\nu_-}{2\sigma_i^3T_o - \sigma_i\varepsilon(2m_+\nu_+ + m_-\nu_- + m_{2-}\nu_{2-})} \tag{E.25}$$

$$S_1 = \frac{\sigma_i[-2\sigma_i^2T_o - (\gamma+\delta)m_-\nu_- + \delta m_{2-}\nu_{2-}]}{2\sigma_i^3T_o - \sigma_i\varepsilon(2m_+\nu_+ + m_-\nu_- + m_{2-}\nu_{2-})} \tag{E.26}$$

$$S_2 = \frac{\gamma}{\sigma_i} \tag{E.27}$$

$$S_3 = \frac{-2\sigma_i^2T_o(\gamma+\delta+\varepsilon) + 2\varepsilon(\gamma+\delta)m_+\nu_+ + 2\delta\varepsilon m_{2-}\nu_{2-} + \gamma\varepsilon m_{2-}\nu_{2-}}{2\sigma_i^3T_o - \sigma_i\varepsilon(2m_+\nu_+ + m_-\nu_- + m_{2-}\nu_{2-})} \tag{E.28}$$

$$S_4 = \frac{2\sigma_1^2 T_0(\delta-\varepsilon) - 2\delta\varepsilon(m_+\nu_+ + m_-\nu_-) - \gamma\varepsilon m_-\nu_-}{\sigma_1^3 T_0 - \sigma_1\varepsilon(2m_+\nu_+ + m_-\nu_- + m_{2-}\nu_{2-})} \tag{E.29}$$

And

$$\frac{N_{2-}}{N_e} = R_1 + S_1 \left(\frac{N_-}{N_e}\right)_{\pm} \tag{E.30}$$

$$\frac{J_e}{N_e} = R_2 + S_2 \left(\frac{N_-}{N_e}\right)_{\pm} \tag{E.31}$$

$$\frac{J_-}{N_e} = R_3 + S_3 \left(\frac{N_-}{N_e}\right)_{\pm} \tag{E.32}$$

$$\frac{J_{2-}}{N_e} = R_4 + S_4 \left(\frac{N_-}{N_e}\right)_{\pm} \tag{E.33}$$

And the characteristic value equation for T_e is

$$\left(\frac{N_-}{N_e} + \frac{N_{2-}}{N_e}\right)\left[-\sigma_1 T_e + m_e\nu_e\left(\frac{J_e}{N_e}\right)\right] - m_-\nu_-\left(\frac{J_-}{N_e}\right) - m_{2-}\nu_{2-}\left(\frac{J_{2-}}{N_e}\right) = F(T_e) = 0 \tag{E.34}$$

Vita

Frank D. Lewis was born 16 July 1944 in Boston, Massachusetts. He graduated from South Side High School in Fort Wayne, Indiana, and attended Purdue University where he graduated with a B.S. in physics in 1967. Subsequently, he entered active duty in the Air Force on 29 September 1967. After receiving his wings in December 1968, he upgraded in F-4 aircraft at George AFB, California. He returned from a tour in F-4's at Ubon Royal Thai AFB in Thailand in October 1969, to fly B-52's for the Strategic Air Command at Mather AFB, California. He flew the B-52 during Arclight from June through December 1972. In July 1973, he was assigned to the 9th Strategic Reconnaissance Wing of SAC at Beale AFB, California. While there, he acted as ground training officer, FAA co-ordinator and refueling monitor, and finally as Chief of Crew Training for the SR-71. He remained at Beale AFB until being reassigned to the Air Force Institute of Technology in June of 1976 in order to pursue an advanced degree in engineering physics.

He is married to the former Wynne G. McCormick and they have one daughter, Kelly, age nine.