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**ELECTRON TRANSPORT COEFFICIENTS AND VIBRATIONAL EXCITATION
RATES FOR ELECTRICALLY EXCITED CO₂ GAS LASERS**

by*

C. J. Elliott, O. P. Judd, A. M. Lockett, and S. D. Rockwood

ABSTRACT

Electron transport coefficients and vibrational excitation rates have been calculated for gas mixtures appropriate for electrically excited CO₂ lasers. The basis of the calculations is a detailed numerical solution of the Boltzmann transport equation which incorporates experimentally determined cross sections for the most important inelastic electron collision processes in the gas. The effects of elastic and superelastic collisions and charged particle interactions have also been included in the formalism. Graphical presentations of electron drift velocity, average energy, characteristic energy, and vibrational excitation rates in a range $10^{16} < E/N < 5 \times 10^{16}$ Vcm² are obtained for nine CO₂-N₂-He gas mixtures. The excitation rates are also presented in a form normalized to average electron energy. Using this normalization, the electron excitation rates for the three vibrational modes in CO₂ are found to be independent of gas mixture within a 20% approximation. The dominant effect of gas mixture on electron kinetic processes is to modify the vibrational excitation rate in the nitrogen. The implication of these results to the basic kinetics of the CO₂ laser is discussed.

I. INTRODUCTION

A knowledge of electron transport coefficients and inelastic excitation rates in a gas influenced by an electric field is necessary for the investigation of electrical discharges and electrical lasers. In particular, a quantitative description for the behavior of CO₂ electrical lasers requires accurate values for the electron drift velocity and vibrational excitation rates over a wide range of operating parameters. The magnitude of these quantities depends on gas mixture and the parameter E/N where E is the electric field and N is the neutral gas density. Since the electron distribution function is generally non-Maxwellian and the inelastic cross sections are strong functions of the electron energy, a self-consistent numerical integration of the Boltzmann transport equation is required to obtain the accurate functional form for the distribution function. The transport coefficients and inelastic excitation rates are then obtained by energy averaging the appropriate cross sections with the calculated distribution function.

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In general, the convolution of the distribution function and inelastic cross sections can be strongly dependent on the gas mixture and E/N . For example in the range of E/N typical of electron beam preionized CO₂ lasers with significant fractions of N₂ in the gas, the excitation rates to the upper laser level are steep functions of E/N . Approximate analytic calculations or small errors in machine computational solutions for the distribution functions can lead to substantial errors in the excitation rate within this range of electron energy. A comparison of theoretical laser kinetics models with experimental data for this type of laser is, therefore, difficult to correlate.

The purpose of this paper is to provide an accurate compendium of electron transport coefficients and vibrational excitation rates, subject only to the accuracy of the electron collision cross sections, for several common gas mixtures employed in CO₂ electrical lasers. The calculations were carried out over a range of E/N that included both the non-sustained and self-sustained discharge regime.

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The data were obtained from numerical solutions to the Boltzmann transport equation. Three independently formulated numerical techniques were employed to provide a cross check of the results and eliminate the possibility of computational errors. In order to provide a best value for the calculated quantities, up-to-date electron impact cross sections have been employed. This aspect of the work is an extension of the earlier work in the field by Frost and Phelps¹, Nighan², and recent work by Lowke *et al.*³ The formulation of the problem is discussed in Section II and the numerical data in Section III. An implicit assumption relating to the accuracy of the data is the validity of the form of the Boltzmann transport equation that is commonly used for these types of calculations. A discussion of this point, the explicit form of the basic equations, and numerical techniques are presented in Appendix A.

A correlation of the computed excitation rates for different gas mixtures has been attempted in order to provide some physical insight into the operation of the CO₂ laser. Scaling parameters have been derived and are discussed in Section IV. A summary of the work is contained in Section V.

II. FORMULATION

The electron distribution function $f(u)$ at energy u is obtained from a numerical integration of the Boltzmann transport equation taking into account the most important elastic and inelastic collision processes that influence the form of $f(u)$. Several forms of the transport equation used for numerical computation and the numerical techniques are summarized in Appendix A. The transport coefficients and inelastic excitation rates are obtained by appropriate integrations over the distribution function in energy space. Gas mixtures consisting of CO₂, N₂, and He are considered.

The electron impact cross sections for vibration and electron excitation and ionization employed in this calculation are those compiled by Phelps and coworkers and are described in detail in reference (3). This reference also contains the cross-section data in tabular form. The explicit cross sections employed in our work are contained in Table I. The elastic and inelastic cross sections for CO₂ are also plotted in Fig. (1). Besides the (010) direct excitation processes, indirect processes that occur

via the CO₂⁻ resonance state⁴, which contribute to excitation of both the bending and symmetric stretch vibration modes of the molecule, are also included. The indirect impact processes are considered according to energy loss, and no interpretation as to the explicit excitation channels within the symmetric-bending mode complex have been attempted. These points are considered in more detail in references (5) and (6). Electron loss due to dissociative attachment is included using the cross section published by Schulz.⁷

The nitrogen inelastic cross sections include vibrational levels $v = 1$ through $v = 8$, the $A^3\Sigma_u^+$, $C^3\Pi_u$, $a^1\Pi_g$, and three unidentified electronic states and ionization as derived by Frost and Phelps.¹ The inelastic cross sections in helium include ionization and a combined cross section for the 2^3S , 2^1S , and 2^1P electronic states.

For completeness, the effects of heavy particle recoil, superelastic collisions, or collisions of the second kind, and electron-ion and electron-electron interactions have been included in the formulation. The magnitude of each of these effects was evaluated numerically with the following results: (a) within the range of E/N considered recoil effects could be neglected except in the case of mixtures with helium fractions greater than 80% in which case recoil effects can dominate the inelastic processes. A gas temperature of 300°K was assumed. (b) superelastic collisions exhibit a negligible effect on the transport coefficients and vibrational excitation rates, but did influence appreciably the quantities determined by the tail of the distribution function such as electron excitation and ionization. Since the inclusion of superelastic processes may significantly increase the computation time and does not contribute significantly to the resulting numerical values for this study, these effects were not included in the computed data discussed in the next section. (c) the effects of charged-particle interactions do not become important until the fractional ionization in the discharge exceeds 10^{-5} for the range of E/N values of interest.⁸ This result can also be verified analytically. Since most CO₂ lasers of interest exhibit a fractional ionization of 10^{-6} , the effects of charged-particle interactions were also neglected in the numerical computations.

The calculated electron transport quantities include the drift velocity v_d , effective average electron energy $\bar{u}$, the characteristic energy u_k , the mobility μ , and the diffusion coefficient D . Following Engelhardt and Phelps⁹ these quantities have been generalized to gas mixtures and are defined by the relations:

$$\mu N = -\frac{1}{3} \left(\frac{2e}{m} \right)^{1/2} \int_0^\infty \frac{u}{\sum_j \psi_j Q_{mj}(u)} \frac{df}{du} du \quad (1)$$

$$v_d = \mu E \quad (2)$$

$$DN = \frac{1}{3} \left(\frac{2e}{m} \right)^{1/2} \int_0^\infty \frac{u f(u)}{\sum_j \psi_j Q_{mj}(u)} du \quad (3)$$

$$u_k = \frac{D}{\mu} \quad (4)$$

$$\bar{u} = \frac{2}{3} \int_0^\infty u^{3/2} f(u) du \quad (5)$$

where e and m are the charge and mass of the electron.

The electron energy u in eV and velocity v are related by $u = \frac{mv^2}{2e}$, and $f(u)$ is normalized such that

$$\int_0^\infty u^{1/2} f(u) du = 1 \quad (6)$$

The momentum transfer cross section for each neutral species j is Q_{mj} . The total cross section is obtained by weighting the individual cross sections by the mole fraction of each species ψ_j and summing over j .

The Maxwellian distribution for electrons at a temperature T_e (eV) subject to the normalization of Eq. (6) is given by

$$f_M = \frac{2}{\sqrt{\pi}} \frac{e^{-u/T_e}}{T_e^{3/2}} \quad (7)$$

The definition of the effective average electron energy given in Eq. (5) then corresponds to the electron energy along the field and for a Maxwellian is just T_e . With a non-Maxwellian distribution the characteristic energy u_k , which is a quantity that can be conveniently determined experimentally, can be compared directly with the calculated effective average energy for a given E/N . In general these two quantities may be quite different for certain gas mixtures, a fact that reflects the non-equilibrium nature of the distribution function.

*From the definition of u , the units of u are volts rather than eV. Since the meaning is usually clear, however, u will be discussed in terms of an energy.

The normalized excitation rate or frequency for the i th inelastic process in species j is defined by

$$\frac{v_{ij}}{N_j} = \left(\frac{2e}{m} \right)^{1/2} \int_0^\infty u f(u) Q_{ij}(u) du \quad (8)$$

where v_{ij}/N_j is given in units of cm^3/sec . An effective average inelastic rate for a collection of levels $\bar{v}$ (e.g., the symmetric-bending complex in CO_2) has also been defined by Nighan² by weighting each inelastic cross section by the inelastic energy loss u_{ij} of the process. In terms of the lowest level of the complex

$$\frac{\bar{v}}{N_j} = \sum_i \frac{v_{ij}}{N_j} \frac{u_{ij}}{u_{1j}} \quad (9)$$

The inelastic loss rate defined in this manner is useful for laser modeling calculations and comparison with other published works in the field.

The calculated data were obtained from three different and independently formulated numerical techniques for solving the Boltzmann transport equation. Given identical input cross sections, the results of the numerical computations were compared at five values of E/N for each calculated quantity. The largest deviations observed were less than 2%. Where comparisons are possible, these results are also within 2% of the published data of Lowke *et al.*³ The method of treating elastic collisions in the numerical code was checked by: (a) inserting a constant momentum transfer cross section of $6 \times 10^{-16} \text{ cm}^2$ for He and comparing the results with that obtained from an analytic solution to the transport equation in the absence of inelastic collision processes. In this limit a Druyvesteyn distribution results. (b) inserting $Q_m \propto u^{-1/2}$, in which case a constant momentum transfer collision frequency is obtained, the analytic solution for the distribution function is a Maxwellian. Comparison of the analytical and numerical results for both the distribution functions and transport coefficients yielded values within 0.5%. The intercomparison provided by the three numerical solutions and the favorable comparison with analytical solutions lends a certain degree of confidence to the numerical integration techniques. The accuracy of the calculated quantities are therefore considered to be limited predominantly by the accuracy of the input electron impact cross sections.

III. TRANSPORT COEFFICIENTS AND EXCITATION RATES

Transport data consisting of the drift velocity, characteristic energy, and average energy are plotted in Fig. (2) through Fig. (9). The mobility can be readily derived from the drift velocity data as can the diffusion coefficient through the use of Eqs. (2) and (4). A comparison of u_k and $\bar{u}$ indicates a near equivalence for mixtures with fractional helium concentrations greater than 0.5. The exception appears to be mixtures with a large N_2 concentration, e.g., 3/2/1. At smaller helium concentrations, the failure of the equivalence of u_k and $\bar{u}$ indicates the error that can be introduced by indiscriminately ascribing an effective temperature to the electron distribution. The effect in N_2 rich mixtures can be understood in terms of the data in pure N_2 shown in Fig. (2). Because of the sharp energy loss barrier introduced into the electron distribution function near the 2-eV resonance in the inelastic vibrational excitation cross section,¹⁰ the value of $\bar{u}$ is relatively insensitive to changes in E/N. The characteristic energy, however, is inversely proportional to the gradient of the distribution function and therefore exhibits a stronger dependence on E/N.

The electron vibrational excitation rates per electron normalized to the species gas density v_j/N_j , are plotted in Figs. (10)-(20) for various gas mixtures. The (010) rate refers to the direct excitation of the (010) level in CO_2 . The effective (NOO + OMO) rate is the sum of all resonant state excitation channels into the combined symmetric-bending mode of CO_2 weighted by the energy of the (010) level. The rate plotted in the graphs is the sum of these two excitation processes and is indicative of the total electron excitation rate into the symmetric-bending mode complex. For purposes of presentation, this rate has been reduced by a factor of 10 in the figures.

The excitation rates in nitrogen have been plotted for each individual vibrational level and also as an energy weighted sum for the first eight vibrational levels. The resulting rates are presented in Figs. (11) and (12).

IV. BASIC SCALING PARAMETERS FOR THE DISTRIBUTION FUNCTION

In order to gain some insight into the physics of the CO_2 laser, it is necessary to separate the

effects due to vibrational kinetics from those due to electron excitation processes under conditions of different gas mixtures and E/N, where N is the total gas pressure. It is therefore desirable to obtain a parameter in terms of which one can plot the vibrational excitation rates and normalize out the dependence on gas mixture. Initial trial choices for such a parameter may be u_k , $\bar{u}$, or E/N_j where N_j could be represented by the N_2 or CO_2 gas density or the sum. Only the first two choices were found to be reasonable in CO_2 - He mixtures; in the presence of nitrogen, only the average energy $\bar{u}$ proved to be a reasonable scaling parameter. The plot of the results for the (001) vibrational excitation rate in CO_2 -He mixtures is shown in Fig. (21). The points represent 5 equal increments of E/N in the range of 1 to 5×10^{-16} Vcm². The scaling with $\bar{u}$ is evident. The results for nitrogen mixtures are plotted in Fig. (22). Also included for comparison is the normalized rate for CO_2 - He mixtures taken from Fig. (21) and is represented by the dotted line in the figure. The effect of the addition of nitrogen is clear in that the rate appears to vary continuously from the dotted curve with small N_2 fractional concentrations to the solid curve if the fractional concentration exceeds 10%. From this data it appears that over the E/N range of interest, the (001) excitation rate appears to depend only on the value of $\bar{u}$ set by a given E/N and to within a 10% approximation is independent of gas mixture. Similarly normalized plots for the (010) direct excitation rate and effective symmetric-bending mode rates are shown in Fig. (23) and Fig. (24). In the absence of N_2 , the data in Fig. (23) indicate that both rates are independent of gas mixture for helium concentrations greater than 0.5. The rate increases about 3% for $\bar{u} > 1$ eV as the helium concentration approaches 1. In the presence of N_2 , both rates are lowered slightly as the N_2 concentration increases. This effect is shown in Fig. (24). Also the normalization with respect to $\bar{u}$ becomes less significant. Comparison of Figs. (23) and (24) shows deviations less than 20% over the complete range of gas mixtures, and within this error, this rate can again be considered to be parameterized by the value of average electron energy in the discharge.

The normalized effective rate for the first eight vibrational levels in nitrogen is plotted in

Fig. (25) as a function of $\bar{u}$ and gas mixture. The value for pure N_2 is shown by the broken curve and has been increased by a factor of two for purposes of presentation. The points indicate ten integral values of E/N in the range of 10^{-16} to 10^{-15} Vcm^2 . In this case the change in the excitation rate with gas mixture for a given $\bar{u}$ is more pronounced. The rate increases by a factor of three in the transition from N_2 fractional concentrations of 1.0 to 0.01. This behavior can be directly attributed to the large resonant inelastic cross section for vibrational excitation at 2.3 eV. The effect of the large cross section is to sharply cut off the distribution function near this electron energy so that most electrons are contained below this energy barrier.¹⁰ Since the vibrational excitation rate is a convolution of the inelastic cross section with the distribution function, in the case of nitrogen, it is obvious that the overlap of the two functions is strongly dependent on the exact form of the distribution function rather than $\bar{u}$, which is an energy average of the electron distribution. This behavior is characteristic of any gas that possesses a large inelastic cross section and reflects the fact that most of the electrons in energy space that are accelerated to high energy by the electric field are returned to low energies by inelastic collisions, and only a small fraction of these electrons penetrate the energy barrier to contribute to the inelastic excitation rate. A similar process has been observed in N_2 and CO where in this case both species possess large inelastic cross sections but are separated by a small internal energy.

The fact that the CO_2 vibrational excitation rates scale with $\bar{u}$ even in the presence of N_2 is due to the even distribution of the inelastic cross sections for these processes in energy space, so the

effect on the distribution function is less pronounced. In N_2 rich mixtures, most of the electrons are contained at energies less than 2.3 eV, so again the scaling with $\bar{u}$ is maintained.

The above results indicate that to good approximation, the rate coefficients for vibration excitation in the CO_2 molecule depend only on the average electron energy in a given gas mixture and not on the mixture itself. Variations in E/N simply rescale the value of $\bar{u}$ in the gas. At a fixed value of $\bar{u}$, the dominant effect of gas mixture variation is to modify the vibrational excitation rate into the nitrogen.

V. SUMMARY

Electron transport coefficients and vibrational excitation rates have been calculated for several gas mixtures in a range of E/N characteristic of CO_2 lasers. Several precautions were taken in obtaining the solution of the Boltzmann Transport equation to insure the accuracy of the numerical results. The effects of superelastic collisions and charged-particle interactions were included in the formulation and were found to be negligible for the included range of E/N and at fractional ionizations less than 10^{-5} .

Within a 20% approximation, the electron excitation rates for the three vibrational modes in CO_2 are found to be independent of gas mixture when normalized to the average electron energy in the different gas mixtures but do not significantly affect the CO_2 vibrational excitation processes or rates at a given average electron energy. The dependence of the vibrational excitation rate in N_2 on gas mixture is much stronger and reflects the dominant effect of changes in the electron distribution function with E/N in a $N_2 - CO_2$ laser discharge.

APPENDIX A

BOLTZMANN EQUATION FORMALISM AND NUMERICAL TECHNIQUES

Three independent formulations were developed for numerical integration of the transport equation. The formulations all begin with a different initial form of the transport equation and employ somewhat different numerical techniques for solving these initial equations. In order to compare these methods, and their relation to other work in the field, the various forms of the Boltzmann equation will be summarized.

The equation for the distribution function $f(v)$ for electrons with velocity v , charge e , and mass m in an electric field E can be written in the form

$$-\frac{e}{m} E \cdot \frac{df(v)}{dv} = \left. \frac{\delta f}{\delta t} \right|_c \quad (A1)$$

where the expression on the right-hand side contains terms that modify $f(v)$ due to elastic, inelastic,

and superelastic electron collision processes. In order to solve (A1), a common method is to expand $f(\underline{v})$ in terms of Legendre polynomials about the direction of the electric field. To lowest order in the electron drift energy $f(\underline{v})$ can be written in the form

$$f(\underline{v}) = f_0(v) + \frac{v}{v} \cdot \underline{f}_1(v). \quad (A2)$$

Under certain conditions, the two-term truncation of this expansion may not be valid. In gases such as N_2 that are characterized by large inelastic cross sections localized in energy space, it has been suggested¹¹ that the value of $\underline{f}_2(v)$ can be as large as $\underline{f}_1(v)$ for values of E/N typical of glow discharges. The effects of higher order terms in the expansion have not yet been evaluated, however. Also, the addition of terms greater than $\underline{f}_1(v)$ requires a knowledge of the angular as well as energy dependence of the inelastic cross sections. Although angular cross-section data are now available for CO_2 and N_2 , we have elected to retain the two-term truncation approximation for $f(\underline{v})$ based on the following justifications: (a) a complete analysis to estimate the magnitude of the error introduced into the calculated values of the transport coefficients and vibrational excitation rates using the two-term truncation is lacking at the present time; (b) the numerical techniques are greatly simplified; (c) many of the cross sections used in the present calculation were determined by fitting measured transport data obtained in pure gases with calculated values obtained from a solution of the Boltzmann equation based on Eq. (A2). Use of these cross sections then dictates use of the same form of the transport equation to calculate the same quantities of interest in gas mixtures.

Substitution of Eq. (A2) into Eq. (A1), multiplying the resulting equation by the first two Legendre polynomials, and integrating with respect to the solid angle, one obtains the well-known result that Eq. (A1) can be written as two first-order coupled equations for $f_0(v)$ and $\underline{f}_1(v)$. The results of this averaging yield

$$-\frac{1}{3} \frac{e}{mv^2} E \cdot \frac{d}{dv} [v^2 \underline{f}_1(v)] = \frac{\delta f_0(v)}{\delta t} \Big|_c \quad (A3)$$

$$-\frac{eE}{m} \frac{df_0(v)}{dv} = \frac{\delta \underline{f}_1}{\delta t} \Big|_c \quad (A4)$$

Assuming that the dominant process responsible for maintaining the isotropy of the zero-order distribution function is that of electron-neutral momentum transfer collisions, the collision term in Eq. (A4) may be written as

$$\frac{\delta \underline{f}_1}{\delta t} \Big|_c = -\sum_j N \psi_j Q_{mj} v \underline{f}_1(v) \quad (A5)$$

where ψ_j is the mole fraction of species j , and Q_{mj} is the momentum transfer cross section for species j . Performing a change of variable to electron energy $u = mv^2/2e$ and substituting Eq. (A4) and Eq. (A5) into Eq. (A3) one obtains

$$\frac{d}{du} (J_f + J_{ek}) = \sum_{ij} \psi_j C_{ij} \quad (A6)$$

where we have defined

$$J_f = -\frac{1}{3} \left(\frac{E}{N} \right)^2 \frac{1}{\sum_j \psi_j Q_{mj}} u \frac{df}{du} \quad (A7)$$

$$J_{ek} = -2u^2 [f + kT \frac{df}{du}] \sum_j \frac{m}{M_j} \psi_j Q_{mj} \quad (A8)$$

$$C_{ij} = (u + u_{ij}) f(u + u_{ij}) Q_{ij}(u + u_{ij}) - u f(u) Q_{ij}(u) + (u - u_{ij}) f(u - u_{ij}) X_{ij} \times Q_{ij}^{(s)}(u - u_{ij}) - u f(u) X_{ij} Q_{ij}^{(s)}(u) \quad (A9)$$

and have normalized $f(u)$ such that $\int_0^\infty u^{1/2} f(u) du = 1$. The quantity J_f is the flux of electrons in energy space driven by the electric field. The recoil effects of the heavy particles of mass M_j during elastic collisions were neglected in Eq. (A5). These corrections have been inserted into Eq. (A6) through the term J_{ek} which can be interpreted as the flux of electrons in energy space driven by elastic collisions. kT is the neutral gas temperature in eV. The effects of inelastic collisions are included in C_{ij} where u_{ij} is the energy loss for the i th inelastic process in species j , and Q_{ij} is inelastic cross section for this process. Inelastic collision of the second kind or superelastic collisions are those terms with cross sections $Q_{ij}^{(s)}$ and are related to Q_{ij} through detailed balance at each energy u . This relation can be expressed in the form¹²

$$Q_{ij}^{(s)}(u) = \left(\frac{u + u_{ij}}{u} \right) Q_{ij}(u + u_{ij}) \quad (A10)$$

X_{ij} is the fractional population of level i in the j th species. Direct substitution of Eqs. (A7), (A8) and (A9) into Eq. (A6) gives the Boltzmann equation

in the explicit form derived by Frost and Phelps,¹ and previously derived in part by Allis,¹³ Holstein,¹⁴ and Carleton and Megill.¹⁵

Three different forms of Eq. (A6) are employed for numerical integration. In the first method (AML), a function $g = -(J_f + J_{el})$ was defined which permits equation (A6) to be written as two coupled differential equations of the form

$$\frac{dg}{du} = - \sum_{i,j} \psi_j C_{ij} \quad (A11)$$

$$\frac{df}{du} = \frac{[g - 2u^2 f \sum \psi_j Q_{mj} m/M_j]}{[\frac{u}{3} (\frac{E}{N})^2 (\sum \psi_j Q_{mj})^{-1} + 2u^2 kT \sum \psi_j Q_{mj} m/M_j]} \quad (A12)$$

The procedure for numerical integration of Eqs. (A11) and (A12) is an iterative method in which collisions of the second kind are treated as a perturbation to the zero-order solutions. This approximation is valid when the vibrational temperature is small compared to the electron temperature. Under these conditions, the rate of electron impact excitation of the vibrational levels greatly exceeds the rate of electron de-excitation so that the latter may be neglected in the first iteration.

The integration is initiated at some large value of energy u_0 and proceeds backwards along the energy axis to $u = 0$. This method is convenient since $f(u + u_{ij})$ can be obtained in a direct manner, and the solution for $f(u)$ is insensitive to the choice of the boundary conditions at u_0 . For reasonable accuracy, u_0 is taken to be in the range $20 T_e \leq u_0 \leq 30 T_e$. The boundary condition on f is that $f(\infty) = 0$. For the purpose of the numerical integration, this condition is approximated by one in which $f(u_0) \ll f(0)$. If $u_0 > 20 T_e$, this condition can be easily satisfied. For convenience, one initially sets $f(u_0) = 1$ and $\frac{df}{du} \Big|_{u=u_0} = L f(u_0)$ where L is the logarithmic derivative of $f(u)$. The choice of L is obtained from a judicious guess for $1/T_e$.

An examination of limiting cases has shown that there exists two independent solutions to the differential equation, an increasing and a decreasing exponential with energy. The latter solution is the desired one. Using the above method, the undesired solution rapidly becomes insignificant as the integration proceeds, and the final solution for $f(u)$ is relatively insensitive to the choice for L if u_0 is chosen sufficiently large. After each integration,

the value of $f(u)$ and $g(u)$ are renormalized in a conventional manner.

The accuracy of the integration is determined by an internal power balance in which the power into the collisional loss processes is compared to the work done by the electric field. Typically this balance is maintained to better than one part in 10^4 . If superelastic collisions are neglected entirely, this accuracy is generally obtained by one integration along the energy axis. The effects of superelastic collisions are obtained by a second integration in which $f(u - u_{ij})$ is calculated using the normalized value of $f(u)$ obtained from the first integration. This process is iterated as many times as necessary to obtain the desired power balance. In general, this procedure will converge rapidly provided the superelastic collisions can be regarded as a perturbation.

The Boltzmann equation also may be rewritten in a somewhat different form in terms of the number density of electrons $n(u)$ between u and $u + du$. In terms of $f(u)$

$$n(u) = N u^{1/2} f(u) \quad (A13)$$

$$\int_0^\infty n(u) du = N$$

Using these definitions, Eqs. (A6), (A7), and (A8) may be cast into the form of a diffusion equation with diffusion coefficient D , and a continuity equation. The resulting coupled equations are:

$$\frac{dn}{du} = \frac{wn - J}{D} \quad (A14)$$

$$\frac{dJ}{du} = N \sum_{i,j} \psi_j C_{ij} \quad (A15)$$

where

$$J = J_f + J_{el} \quad (A16)$$

$$w = \left[\frac{1}{6u} \left(\frac{E}{N} \right)^2 \left(\sum \psi_j Q_{mj} u^{1/2} \right)^{-1} - \right.$$

$$\left. \left(u - \frac{kT}{2} \right) \frac{2}{N} \sum \frac{m}{M_j} \psi_j Q_{mj} u^{1/2} \right] \quad (A17)$$

$$D = \left[\frac{1}{3} \left(\frac{E}{N} \right)^2 \left(\sum \psi_j Q_{mj} u^{1/2} \right)^{-1} + \frac{2u}{N} \frac{3/2}{kT} \right] \quad (A18)$$

The time-dependent generalization of this form of the transport equation was essentially derived by Zeldovich and Raizer.¹⁶ Eqs. (A14) through (A18) constitute the working equations for the second (CJE) numerical scheme. The boundary conditions imposed

on the equations are $n(u_0) = 1$ and $J(u_0) = 0$. Using the methods described previously and a predictor-corrector integration scheme, the equations are integrated from some value of u_0 to $u = 0$. The dominant difference between the AML and CJE methods is the different functional form used for the coupled equations.

The third (SDR) method uses a basically different numerical technique than the previous ones. The working equations are of the form of (A6), (A7), (A8) and (A9) rewritten in terms of $n(u)$. Equation (A6) is converted to a set of K-coupled, ordinary differential equations by finite differencing the electron energy axis into K cells of width Δu . The details of the numerical procedure are contained in reference (8) and (17) and will not be repeated here. This form of the equation is particularly convenient for treating the effects of superelastic and electron-electron collisions.

In the absence of superelastic collisions or charged-particle interactions, the numerical integration of the Boltzmann equation and evaluation of the transport coefficients and excitation rates proceeds rapidly. For each value of E/N , the first and second methods require 15-30 seconds of CDC-7600 computer time to achieve an internal power balance of one part in 10^4 . The third method is somewhat faster and typically achieves the same result in 4 seconds.

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Table I. Electron impact cross sections for the elastic and inelastic processes considered in the computation. All cross sections are presented in units of 10^{-16} cm^2 .

MOMENTUM TRANSFER CROSSSECTIONS (10^{-16} CM^2)			
ENERGY (E-VOLTS)	HE CROSSSECTION	N2 CROSSSECTION	CO2 CROSSSECTION
0.000	4.960	1.000	600.000
.001	4.980	1.340	540.000
.002	5.020	1.490	380.000
.003	5.070	1.620	325.000
.005	5.120	1.810	247.000
.007	5.150	2.000	200.000
.009	5.180	2.100	185.000
.010	5.210	2.190	170.000
.015	5.280	2.550	145.000
.020	5.350	2.850	120.000
.030	5.460	3.400	102.500
.040	5.540	3.860	85.000
.050	5.620	4.330	79.000
.070	5.740	5.130	64.000
.100	5.860	6.000	52.000
.150	6.040	7.120	40.000
.200	6.160	7.450	31.500
.250	6.270	8.500	25.000
.300	6.350	8.800	20.000
.350	6.420	9.440	16.500
.400	6.490	9.700	13.000
.500	6.590	9.950	7.700
.700	6.730	9.980	6.300
1.000	6.850	9.980	5.600
1.200	6.910	10.510	5.200
1.300	6.920	11.000	5.100
1.500	6.960	11.960	5.000
1.700	6.970	13.430	5.000
1.900	6.980	19.830	5.100
2.100	6.980	26.380	5.300
2.200	6.980	28.760	5.400
2.500	6.960	29.600	6.500
2.800	6.920	28.010	7.600
3.000	6.890	21.630	9.000
3.300	6.820	17.190	11.300
3.600	6.730	14.660	14.200
4.000	6.600	12.620	15.200
4.500	6.490	11.520	14.800
5.000	6.260	11.100	13.200
6.000	6.010	10.300	10.300
7.000	5.530	10.200	10.200
8.000	5.240	9.900	10.800
10.000	4.450	9.510	12.100
12.000	4.020	10.140	13.100
15.000	3.580	11.100	14.500
17.000	3.350	11.300	15.200
20.000	3.050	12.000	15.700
25.000	2.710	11.700	16.000
30.000	2.450	11.100	16.000
50.000	2.860	9.300	13.000
75.000	1.400	7.700	9.600
200.000	1.150	6.600	8.000

Table I.

INELASTIC CROSSSECTIONS FOR HELIUM
(10^{-16} CM²)

ENERGY (E-V)	CROSSSECTION EXCITATION LOSS= 19.8	ENERGY (E-V)	CROSSSECTION IONIZATION LOSS= 24.6
0.0000	0.0000	0.0000	0.0000
19.8000	0.0000	24.6000	0.0000
20.0200	.0410	30.0000	.0710
20.2400	.0460	34.0000	.1210
21.4500	.0420	40.0000	.1780
21.8000	.0550	45.0000	.2120
22.4500	.0550	50.0000	.2420
24.2200	.0730	60.0000	.2890
25.3200	.0920	70.0000	.3130
27.5300	.1080	80.0000	.3320
29.7500	.1160	90.0000	.3440
34.1800	.1210	100.0000	.3510
46.3000	.1210	150.0000	.3460
100.0000	.1150	200.0000	.3240
200.0000	.1000		

VIBRATION CROSSSECTIONS FOR NITROGEN
(10^{-16} CM²)

ENERGY (E-V)	CROSSSECTION V=1 LOSS= .290	ENERGY (E-V)	CROSSSECTION V=2 LOSS= .590	ENERGY (E-V)	CROSSSECTION V=3 LOSS= .880
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
.2900	0.0000	.5900	0.0000	.8800	0.0000
.3000	0.0000	1.7000	0.0000	1.7000	0.0000
.3300	.0020	1.8000	.0900	1.8000	0.0000
.4000	.0030	1.9000	.4000	1.9000	.1800
.7500	.0050	2.0000	1.5200	2.0000	.7500
.9000	.0065	2.1000	1.4800	2.1000	1.4100
1.0000	.0080	2.2000	.6200	2.2000	1.6900
1.1000	0.0000	2.3000	.6000	2.3000	.9500
1.1650	.0120	2.4000	1.3900	2.4000	.2900
1.2000	.0137	2.5000	1.1400	2.5000	.7700
1.2180	.0150	2.6000	.3100	2.6000	1.1700
1.4000	.0675	2.7000	.4900	2.7000	.6400
1.5000	.0950	2.8000	.5100	2.8000	.2600
1.6000	.1220	2.9000	.1800	2.9000	.4000
1.6500	.1300	3.0000	.2400	3.0000	.4000
1.7000	.1600	3.1000	.1500	3.1000	.1600
1.8000	.3300	3.2000	.1100	3.2000	.1600
1.9000	1.5200	3.3000	.0700	3.3000	.1600
2.0000	1.3200	3.4000	0.0000	3.4000	0.0000
2.1000	.4600	20.0000	0.0000	20.0000	0.0000
2.2000	1.6300	150.0000	0.0000	150.0000	0.0000
2.3000	1.2300				
2.4000	.4600				
2.5000	.8600				
2.6000	1.0400				
2.7000	.2700				
2.8000	.4200				
2.9000	.4270				
3.0000	.4300				
3.1000	.5800				
3.2000	.3800				
3.3000	.2900				
3.6000	.2900				
5.0000	0.0000				
150.0000	0.0000				

Table I.

VIBRATION CROSSSECTIONS FOR NITROGEN
(10**-16 CM**2)

ENERGY (E-V)	CROSSSECTION V=4 LOSS=1.170	ENERGY (E-V)	CROSSSECTION V=5 LOSS=1.470	ENERGY (E-V)	CROSSSECTION V=6 LOSS=1.760
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1.1700	0.0000	1.4700	0.0000	1.7000	0.0000
1.7000	0.0000	1.7000	0.0000	1.7000	0.0000
1.8000	0.0000	1.8000	0.0000	1.8000	0.0000
1.9000	0.0000	1.9000	0.0000	1.9000	0.0000
2.0000	.1600	2.0000	0.0000	2.0000	0.0000
2.1000	.4600	2.1000	.2000	2.1000	0.0000
2.2000	1.1000	2.2000	.4600	2.2000	0.0000
2.3000	1.3000	2.3000	.7700	2.3000	.1100
2.4000	.7100	2.4000	1.0400	2.4000	.3700
2.5000	.2000	2.5000	1.0100	2.5000	.6000
2.6000	.3100	2.6000	.5100	2.6000	.6000
2.7000	.6000	2.7000	.2700	2.7000	.3700
2.8000	.4900	2.8000	.3700	2.8000	.1500
2.9000	.1800	2.9000	.6200	2.9000	.0900
3.0000	.1600	3.0000	.4200	3.0000	.1600
3.1000	.1600	3.1000	.2700	3.1000	.1800
3.2000	.1100	3.2000	.3500	3.2000	.0700
3.3000	.0700	3.3000	.3100	3.3000	.0500
3.4000	0.0000	3.4000	0.0000	3.4000	0.0000
20.0000	0.0000	20.0000	0.0000	20.0000	0.0000
150.0000	0.0000	150.0000	0.0000	150.0000	0.0000

VIBRATION CROSSSECTIONS FOR NITROGEN
(10**-16 CM**2)

ENERGY (E-V)	CROSSSECTION V=7 LOSS=2.060	ENERGY (E-V)	CROSSSECTION V=8 LOSS=2.350	ENERGY (E-V)	CROSSSECTION V=9 LOSS=5.000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2.0600	0.0000	2.3500	0.0000	5.0000	0.0000
2.1000	0.0000	2.5000	0.0000	5.7000	.4000
2.1400	0.0000	2.6000	.0700	5.8000	.4200
2.1800	0.0000	2.7000	.1100	6.1000	.4200
2.2200	0.0000	2.8000	.1800	6.2000	.4000
2.2600	0.0000	2.9000	.2400	7.0000	.0600
2.3000	0.0000	3.0000	.1500	9.0000	0.0000
2.4000	.0700	3.1000	.0700	20.0000	0.0000
2.5000	.1800	3.2000	0.0000	150.0000	0.0000
2.6000	.2900	3.3000	0.0000		
2.7000	.4400	3.4000	0.0000		
2.8000	.3300	20.0000	0.0000		
2.9000	.1800	150.0000	0.0000		
3.0000	.0500				
3.1000	.0700				
3.2000	.1600				
3.3000	.0700				
3.4000	0.0000				
20.0000	0.0000				
150.0000	0.0000				

INELASTIC CROSSSECTIONS FOR NITROGEN
(10**-16 CM**2)

ENERGY (E-V)	CROSSSECTION A3SIP LOSS= 6.70	ENERGY (E-V)	CROSSSECTION A1PG LOSS= 0.40	ENERGY (E-V)	CROSSSECTION C3PU LOSS=11.20
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6.7000	0.0000	0.4000	0.0000	11.2000	0.0000
7.1000	.5000	6.7000	.4200	13.5000	.4400
7.3000	.5600	9.0000	.4200	14.0000	1.0000
8.0000	.5600	10.0000	.3000	14.5000	1.0000
8.3000	.5000	20.0000	0.0000	15.1000	.2400
8.7000	.2400	150.0000	0.0000	20.5000	.2200
9.5000	.1000			100.0000	.0500
20.0000	0.0000				
150.0000	0.0000				

Table I.

INELASTIC CROSSSECTIONS FOR NITROGEN
(10⁻¹⁶-16 CM²)

ENERGY (E-V)	CROSSSECTION ELECTRONIC LOSS=12.50	ENERGY (E-V)	CROSSSECTION ELECTRONIC LOSS=14.00	ENERGY (E-V)	CROSSSECTION IONIZATION LOSS=15.50
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12.5000	0.0000	14.0000	0.0000	15.5000	0.0000
13.0000	.4000	14.2000	1.3000	16.5000	.0346
13.5000	.4000	14.4000	1.7000	16.7000	.0408
14.0000	.1600	14.7000	1.7000	17.1100	.0513
20.0000	0.0000	15.0000	.2000	16.6000	.1161
150.0000	0.0000	20.5000	.2000	20.0000	.2010
		25.5000	2.6000	23.0000	.4400
		150.0000	2.8000	25.0000	.6160
				26.0000	.8800
				30.0000	1.0490
				34.0000	1.3600
				37.0000	1.5730
				40.0000	1.7720
				43.0000	1.9440
				46.0000	2.0880
				48.0000	2.1660
				50.0000	2.2270
				54.0000	2.3700
				60.0000	2.5300
				65.0000	2.6200
				70.0000	2.7000
				75.0000	2.7600
				80.0000	2.8100
				85.0000	2.8500
				90.0000	2.8700
				95.0000	2.8900
				100.0000	2.9000

VIBRATION CROSSSECTIONS FOR CO2
(10⁻¹⁶-16 CM²)

ENERGY (E-V)	CROSSSECTION vib LOSS= .083	ENERGY (E-V)	CROSSSECTION 020+100 LOSS= .167	ENERGY (E-V)	CROSSSECTION 0N0+000 LOSS= .252
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
.0827	0.0000	.1670	0.0000	.2520	0.0000
.0844	.0500	.2000	.6000	1.5000	0.0000
.0862	1.1000	.2200	.7600	1.9500	0.0000
.0932	1.8500	.2500	.8000	2.5000	0.0000
.1035	2.3000	.3000	.7800	3.0000	.9200
.1200	2.6000	.5000	.6400	3.5000	.5400
.1302	2.6800	.7000	.5300	4.1000	.3400
.1726	2.6700	1.0000	.4400	4.5000	.1600
.2070	2.4800	1.2500	.4400	5.0600	.6440
.2750	2.1800	1.5000	.4400	6.0000	0.0000
.3450	1.9300	2.0000	.5300	100.0000	0.0000
.5000	1.4500	2.5000	.8400		
.7000	1.1000	3.0000	1.2800		
.9000	.8000	3.2000	1.5700		
1.1000	.6700	3.4000	1.7700		
1.4000	.4600	3.5500	1.7800		
1.6000	.4200	3.7000	1.7500		
1.8000	.4400	3.9000	1.6000		
2.3000	.7000	4.1000	1.2800		
2.4000	.9300	4.5000	.8800		
3.0000	1.3400	4.9000	.3900		
3.2000	1.5800	5.2000	.3300		
3.4000	1.7500	6.0000	.2700		
3.6000	1.6000	8.0000	.2500		
3.8000	1.7900	10.0000	.2100		
4.0000	1.7000	20.0000	0.0000		
4.2000	1.5200	100.0000	0.0000		
4.4000	1.0500				
5.1000	.5700				
5.5000	.5100				
6.0000	.5000				
7.0000	.4800				
8.0000	.4500				
10.0000	.2000				
20.0000	0.0000				
50.0000	0.0000				
100.0000	0.0000				

Table I.

VIBRATION CROSSSECTIONS FOR CO₂
(10**+16 CM**2)

ENERGY(E-V)	CROSSSECTION 001 LOSS= .291	ENERGY(E-V)	CROSSSECTION 0N0+N00 LOSS= .339	ENERGY(E-V)	CROSSSECTION 0N0+N00 LOSS= .422
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
.2910	0.0000	.3390	0.0000	.4220	0.0000
.2970	.4000	1.5000	0.0000	1.5000	0.0000
.3030	.5000	1.9500	.0700	1.9500	0.0000
.3270	.6200	2.5000	.2000	2.5000	0.0000
.3640	.7100	3.0000	.4100	3.0000	.1050
.4250	.7700	3.5600	.6600	3.5600	.2250
.4850	.8400	4.1000	.3400	4.1000	.1000
.6070	.9200	4.5000	.1550	4.5000	0.0000
.7280	.9700	5.0600	0.0000	5.0600	0.0000
.9690	.9900	6.0000	0.0000	6.0000	0.0000
1.2100	.9500	100.0000	0.0000	100.0000	0.0000
2.4300	.6600				
4.8500	.4400				
9.6800	.2600				
18.2000	.1500				
36.4000	.0920				
58.2000	.0540				
100.0000	0.0000				

VIBRATION CROSSSECTIONS FOR CO₂
(10**+16 CM**2)

ENERGY(E-V)	CROSSSECTION 0N0+N00 LOSS= .505	ENERGY(E-V)	CROSSSECTION 0N0+N00 LOSS=2.500
0.0000	0.0000	0.0000	0.0000
.5050	0.0000	2.5000	0.0000
1.5000	0.0000	3.0000	.1400
1.9500	0.0000	3.6000	.2500
2.5000	0.0000	4.1000	.1400
3.0000	.1560	4.5000	0.0000
3.5600	.3300	100.0000	0.0000
4.1000	.1560		
4.5000	0.0000		
5.0600	0.0000		
6.0000	0.0000		
100.0000	0.0000		

INELASTIC CROSSSECTIONS FOR CO₂
(10**+16 CM**2)

ENERGY(E-V)	CROSSSECTION CO+O- LOSS= 3.85	ENERGY(E-V)	CROSSSECTION ELECTRONIC LOSS= 7.00
0.0000	0.0000	0.0000	0.0000
3.8500	0.0000	7.0000	0.0000
4.3000	.0014	8.0000	.6000
4.5000	.0014	8.5000	.6000
5.1000	0.0000	11.0000	0.0000
6.6000	0.0000	100.0000	0.0000
7.2000	.0007		
8.2000	.0045		
8.4000	.0042		
8.9000	.0010		
9.7000	0.0000		
100.0000	0.0000		

Table 1.

INELASTIC CROSSSECTIONS FOR CO₂
(10⁻¹⁶-16 CM²)

ENERGY (E-V)	CROSSSECTION ELECTRONIC LOSS=10.50	ENERGY (E-V)	CROSSSECTION IONIZATION LOSS=13.10
0.0000	0.0000	0.0000	0.0000
10.5000	0.0000	13.3000	0.0000
12.0000	.6900	14.5000	.0600
12.7000	.7300	15.0000	.1000
13.5000	.7800	16.0000	.1800
15.0000	.8800	18.0000	.3540
17.0000	1.0400	20.0000	.5320
20.0000	1.2400	30.0000	1.0000
40.0000	3.6000	40.0000	2.2800
100.0000	6.3000	50.0000	2.7900
		70.0000	3.4300
		100.0000	3.7400

Fig. 1. Momentum transfer and inelastic scattering cross sections for electrons in CO₂ (Reference 3).

Fig. 2.

Fig. 2-10. Electron drift velocity, average energy, and characteristic energy as a function of E/N for $\text{He-N}_2\text{-CO}_2$ gas mixtures.

Fig. 3.

Fig. 4.

Fig. 5.

Fig. 6.

Fig. 7.

Fig. 8.

Fig. 9.

FIG. 10.

Fig. 11.

Figs. 11-20. Electron impact excitation rates for several vibration modes in He-N₂-CO₂ gas mixtures as a function of E/N. The mode designations are discussed in the text. The numerical value for the (NOO + OMO) rate obtained from the graph should be multiplied by a factor of 10.

Fig. 12.

Fig. 13.

Fig. 14.

Fig. 15.

Fig. 16.

Fig. 17

Fig. 18.

Fig. 19.

Fig. 20.

Fig. 21. Electron excitation rate for the (001) asymmetric vibrational level in CO_2 as a function of average electron energy for several He- CO_2 gas mixtures.

Fig. 22. Electron excitation rate for the (001) asymmetric vibrational level in CO_2 as a function of average electron energy for several He- N_2 - CO_2 gas mixtures.

Fig. 23. Electron excitation rates for the (010) and (N00 + 0m0) vibrational levels in CO_2 as a function of average electron energy for several He- CO_2 gas mixtures.

Fig. 24. Electron excitation rates for the (010) and (N00 + 0m0) vibrational levels in CO_2 as a function of average electron energy for several He- N_2 - CO_2 gas mixtures.

Fig. 25. Total electron excitation rate for the first 8 vibrational levels in N_2 as a function of average electron energy for several He- N_2 - CO_2 gas mixtures.