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# Predictions of Microwave Breakdown in Air from Kinetic Theory Calculations

Prepared by CARL J. LENANDER  
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June 1968

Laboratory Operations  
AEROSPACE CORPORATION

Prepared for SPACE AND MISSILE SYSTEMS ORGANIZATION  
AIR FORCE SYSTEMS COMMAND  
LOS ANGELES AIR FORCE STATION  
Los Angeles, California

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## ABSTRACT

A formulation of the Boltzmann equation for dc and microwave electric field excitation in a uniform, multicomponent gas has been expressed in a computer program at the National Bureau of Standards by L. R. Megill. This program was intended for use in the study of atmospheric afterglow by NBS but was given to the Aerospace Corporation for conversion to study microwave breakdown. The conversion of the program, the alteration of the collision cross-section data pack, and the numerical verification that the program plus data pack accurately describe the response of air to high intensity microwaves are described in this report.

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## I. INTRODUCTION

Prediction of the electrical breakdown of any gas requires a knowledge of the relationship between the net ionization frequency and the applied electric field. Data establishing this relationship have been acquired for both ac and dc fields in a variety of gases. Successful theoretical prediction of this relationship has been restricted to the rare gases because of the complexity of the Boltzmann equation, which is used to describe the behavior of the gas under the influence of an electric field. The computational problems associated with a complex gas having many energy levels may be avoided for the rare gases having only a few excitation processes in addition to the elastic and ionization collision processes. For a diatomic gas such as air at low temperatures, the multitude of rotational, vibrational, and electronic excitation processes greatly complicates the problem.

However, a few years ago Carleton and Megill (Ref. 1) at the National Bureau of Standards (NBS) developed a computer program for studying dry air under atmospheric conditions. Their studies were limited to electronic state excitation processes that required field strengths well below breakdown levels. The application of their program to breakdown conditions was later performed by Lombardini (Ref. 2). His report was limited in that a detailed comparison of the theoretically predicted and experimentally observed net ionization frequencies was not presented. Such a comparison would be valuable as an aid to interpretation of current methods of presenting retained experimental results.

The Carleton and Megill program was a sound analysis, but the output of the program would benefit considerably from improvement of the electron collision cross sections that were input to the program. Since the time of the original compilation of the data pack, the accuracy of the experimental cross sections has improved considerably. Also, the role of importance of the different inelastic processes shifts as the average energy of the electrons increases. For these reasons, the data pack was completely updated. Some cross sections were added, especially in the electronic excitation energy region, which is of prime importance in the prebreakdown gas energy distribution. In all cases, the most recently determined or highest confidence values were used.

Solutions of the Boltzmann equation were obtained for various mixtures of  $O_2$  and  $N_2$  over a range of total densities with ac and dc driving fields ranging from below breakdown to substantially above breakdown. The principal results are: the electron distribution function, average energy, mobility, diffusion coefficient, and excitation frequencies for the various molecular states including the total collision, ionization, and attachment frequencies.

## II. THE BOLTZMANN EQUATION SOLVED

The derivation of the Boltzmann equation is covered in detail in the original Carleton and McGill (Ref. 1) article and a variety of other sources (Ref. 2) and will not be presented here. The derivation starts with the Boltzmann equation for spatially uniform electron distributions  $f(\vec{v}, t)$

$$\frac{df}{dt} + \vec{a} \cdot (\vec{\nabla}_{\vec{v}} f) = \left(\frac{df}{dt}\right)_{\text{coll}} \quad (1)$$

where  $\vec{a}$  is the acceleration due to the driving force and  $\vec{\nabla}_{\vec{v}}$  is the gradient in velocity ( $\vec{v}$ ) space. The solution is assumed to have the form

$$f(\vec{v}) = f_0(\vec{v}) + \vec{E} \cdot \vec{v} f_1(\vec{v}) + (\vec{B} \times \vec{E}) \cdot \vec{v} f_2(\vec{v})$$

where  $\vec{E}$  and  $\vec{B}$  are the electric and magnetic fields, respectively. An expansion of  $f(\vec{v})$  in spherical harmonics in  $\vec{v}$  space results in the following equation:

$$\frac{dg}{du} = -\sum_I \frac{m^2 N_1}{(eE)^2 \alpha(u) k} \left\{ \frac{3}{2} \frac{m}{M_1} \sqrt{\frac{u}{k}} \sigma_{1c}(u) g(u) + \frac{12kW_1 \sigma_{1r}(u)}{m\sqrt{u}} g(u) \right. \\ \left. + \frac{0.75}{\sqrt{ku}} \sum_I \int_0^u \left[ (u + u_{1j}) \sigma_{1j}(u + u_{1j}) g(u + u_{1j}) - u \sigma_{1j}(u) g(u) \right] du \right\} \quad (2)$$

where  $E$  is the rms amplitude of the electric field with angular frequency  $\omega$ ,  $g(u) = f_0(u)$ ;  $u(\text{eV}) = kv^2$ , where  $k$  is the units conversion factor;  $(e/m)$  is the electron charge to mass ratio;  $N_1$  is the density of species 1 with mass  $M_1$ , which has an elastic cross section  $\sigma_{1c}(u)$ , an average rotational cross section of  $\sigma_{1r}$ , and inelastic processes  $j$  described by  $\sigma_{1j}(u)$  with threshold energies  $u_{1j}(\text{eV})$ .  $W_1$  is the average energy loss in a rotational collision process with species 1. The expressions for  $f_1(u)$  and  $f_2(u)$  are given in terms of  $f_0(u)$  or  $g(u)$  as

$$f_1(u) = -\frac{2ke}{m} \alpha(u) \frac{dg}{du} \quad (3)$$

$$f_2(u) = \frac{\Omega}{v(u)} f_1(u) \quad (4)$$

where  $\Omega = (eB/m)$ ,

$$\alpha(u) = \frac{v(u) (\omega^2 + \Omega^2 + v^2(u))}{(\omega^2 - \Omega^2) + v^4(u) + 2v^2(u) (\omega^2 + \Omega^2)} \quad (5)$$

$$v(u) = \sum_{ij} N_{ij} \sqrt{\frac{u}{k}} \left[ \sigma_{ic}(u) + \sigma_{iv}(u) + \sigma_{ij}(u) \right] \quad (6)$$

The valid solutions for large field strengths are limited to small fractions of  $f_1/f_0$  and  $f_2/f_0$ .

In the driving frequency domain, either the solutions are limited to

$$\frac{1}{\omega} \ll \int_{u_{av}}^{0.4u_{av}} \frac{du}{\delta(u)\omega v(u)} = \text{relaxation time} \quad (7)$$

where  $\delta(u)$  is the average fractional energy loss of an electron per collision at energy  $u$ , or  $\omega$  may be zero. Thus, there is a low driving frequency region that would produce solutions of questionable validity. An alternate expression (Ref. 3) requires that

$$\frac{e}{m} \cdot \frac{v/\omega}{\left[1 + \left(\frac{v}{\omega}\right)^2\right]} \left(\frac{E}{\omega}\right)^2 g(u)$$

be small. Roughly, this expression means that  $(e/m)(E/\omega)^2$  be small. Spatial gradients are negligible provided

$$1 > 2E \frac{\lambda}{\langle u \rangle} + \frac{\lambda}{\Lambda}$$

where  $\lambda$  is the electron mean free path,  $\langle u \rangle$  is the average electron energy, and  $\Lambda$  is the diffusion length.

Further discussion of the limits of the theory in relation to observable quantities may be found in MacDonald's (Ref. 3) consideration of the limits of diffusion theory.

### III. CALIBRATION OF THE COMPUTER PROGRAM

Frequently, computer programs are written and used on complex problems without any attempt to solve a classical problem that is analytically tractable. Such an exactly solvable problem should always be the first result of the program in order to establish a reference of accuracy for the solution mechanism.

The Maxwellian distribution is an exact solution of the Boltzmann equation with the collision frequency equal to a constant. This problem was solved by the routine and produced numerical representations of the Maxwellian accurate to four places as checked by use of a standard four-place table (Ref. 4); the actual solution may be many places more accurate.

A solution similar to a Maxwellian, but with an average energy given by  $kT + (\text{const}) E^2$  where  $k$  is the Boltzmann constant and  $T$  is temperature, results when the constant collision frequency problem has a dc electric field of strength  $E$  applied. This solution was also obtained to at least four places.

Further calibration of the program to include the data pack will be presented in Section VI.

#### IV. IONIZATION

In breakdown studies, the production of free electrons by ionization is the single most important electron production mechanism. The original NBS program and a similar program developed at Westinghouse by Phelps treat the ionization process the same as any inelastic excitation process in that the primary electron is considered to have lost an amount of energy equal to the threshold energy  $E_T$  and the secondary electron is ignored.

Actually, the two electrons resulting from the ionization are free, and they share the energy of the primary electron. The two resultant electrons are indistinguishable and individually may have energies ranging from zero to  $E - E_T$  ( $E$  = energy of the primary electron). In the Aerospace version of the program, it is assumed that the resultant electrons share the available energy. That is, they each reenter the electron distribution at an energy  $\frac{1}{2}(E - E_T)$ . This choice represents an average in the available energy distribution between the two electrons for the case of reasonably low impact energies as encountered in the breakdown environment. Or, it may be stated that it is highly unlikely that one electron acquires all the available energy in the ionization process and the other electron none.

## V. CROSS-SECTION DATA

The cold-air data pack cross sections in  $O_2$  and  $N_2$  over the energy range from 0 - 20 eV are those described in Ref. 5 but edited to eliminate processes of minimum importance to the breakdown problem. The cross sections used in the data pack are listed in Table I in their order of occurrence in the program. For the most part, the determinations of Phelps (Ref. 6), Schulz (Ref. 7), Chen (Ref. 8), and Rapp and Briglia (Ref. 9) have been relied upon heavily. The exception is the  $O_2$  elastic cross section, which is obtained by transformation properties from  $N_2$  as described in Ref. 5.

The best confidence that can be ascribed to some of the cross sections is  $\pm 5\%$ , and the worst is  $\pm 20\%$ . These confidences are the estimates of Phelps (Ref. 6) and are, to a certain extent, arbitrary. For the study of breakdown and prebreakdown, the most arbitrary portion of the data pack is comprised of the "lumped electronic" excitation cross sections. This is due to the fact that the electronic states that are "lumped" lie in just the energy range forming the last "energy loss barrier" or energy loss mechanism, which keeps the tail of the electron distribution from rising in value in the energy range of the ionization process. The rising in the tail of the distribution function results in an increase in the ionization rate.

Table I. Air Data Pack Cross-Section Composition<sup>a</sup>

Species	ID No.	Cross Section	Threshold (eV)	Energy Loss (u=energy)
O <sub>2</sub>	1	Elastic	0	$2m_e u/M_{O_2}$
O	2	Elastic	0	$2m_e u/M_O$
N <sub>2</sub>	3	Elastic	0	$2m_e u/M_{N_2}$
Blank	4			
N <sub>2</sub>	5	Rotational		$2.49 \times 10^{-4}$
Blank	6			
N <sub>2</sub>	7	X - c <sup>3</sup> $\pi_u$	11.2	11.2
O <sub>2</sub>	8	vib	0.196	0.196
Blank	9			
Blank	10			
Blank	11			
O <sub>2</sub>	12	X - a <sup>1</sup> $\Delta_g$	0.98	0.98
O <sub>2</sub>	13	X - b <sup>1</sup> $\Sigma_u^+$	1.65	1.65
O <sub>2</sub>	14	X - A <sup>3</sup> $\Sigma_u^+$	4.47	4.47
O <sub>2</sub>	15	X - B <sup>3</sup> $\Sigma_u^-$	6.17	6.17
O <sub>2</sub>	16	Lumped elect	9.5	9.5
O <sub>2</sub>	17	Dissoc att	4.0	4.0
O <sub>2</sub>	18	Ionization	12.2	0.5(u - 12.2)
O	19	<sup>3</sup> P - <sup>1</sup> D	1.96	1.96
O	20	<sup>3</sup> P - <sup>1</sup> S	4.17	4.17
O	21	Lumped elect	9.5	9.5
O	22	Ionization	13.6	0.5(u - 13.6)
N <sub>2</sub>	23	$\nu = 0 - 1$	0.29	0.29
N <sub>2</sub>	24	0 - 2	1.70	1.70
N <sub>2</sub>	25	0 - 3	1.80	1.80
N <sub>2</sub>	26	0 - 4	2.0	2.0

<sup>a</sup>From Ref. 5.

Table I. Air Data Pack Cross-Section Composition (Concluded)

Species	ID No.	Cross Section	Threshold (eV)	Energy Loss (u=energy)
N <sub>2</sub>	27	0 - 5	2.0	2.0
N <sub>2</sub>	28	0 - 6	2.2	2.2
N <sub>2</sub>	29	0 - 7	2.4	2.4
N <sub>2</sub>	30	0 - 8	2.6	2.6
N <sub>2</sub>	31	X - A <sup>3</sup> <sub>Σ<sub>u</sub></sub>	6.7	6.7
N <sub>2</sub>	32	X - B <sup>3</sup> <sub>Π<sub>g</sub></sub>	7.39	7.39
N <sub>2</sub>	33	X - a <sup>1</sup> <sub>Π<sub>g</sub></sub>	8.4	8.4
N <sub>2</sub>	34	Lumped elect	5.0	5.0
N <sub>2</sub>	35	Phelps 14 eV	14.	14.
N <sub>2</sub>	36	Ionization	15.58	0.5(u - 15.58)

## VI. DC CALIBRATION

The final data pack, as described in Table I and in Section V, was used in a calibration sequence to establish confidence in future calculations. The standard for calibration was Phelps'  $N_2$  results in a dc field. Phelps' (Ref. 6) results closely follow the experimental drift tube measurements, thus giving the present calibration a reference to experimental values.

Because the underlying interest in this study is in breakdown and prebreakdown field strengths, the calibration to Phelps' (Ref. 6) results was limited to this regime. The test conditions were at a temperature of  $77^\circ\text{K}$  with  $E/N$  values of 1, 2, 3, 4, and  $5 \times 10^{-15} \text{ V-cm}^2$ . Comparison was made with Phelps' (Ref. 6) curve of ionization coefficient  $\alpha_1/N$  vs  $E/N$ , where  $N$  is the gas density (Ref. 6, Fig. 7), and with his distribution function for  $E/N = 3 \times 10^{-15} \text{ V-cm}^2$  (Ref. 6, Fig. 8).

Calculation of  $\alpha_1 = \nu_1 w$ , where  $\nu_1$  is the ionization frequency and  $w$  is the drift velocity, was made for a range of  $E/N$  values. Values of Phelps' characteristic energy  $\epsilon_K$ ,  $w$ , and  $\alpha_1$  were compared with Phelps' published curves (Ref. 6). The agreement was within the same error as Phelps' results with respect to the experimental values and was as close as was readable from the graphs (Figs. 1 and 2). Similarly, the distribution function for the case  $E/N = 3 \times 10^{-15} \text{ V-cm}^2$  was as close to Phelps' results (Ref. 6, Fig. 8) as could be read from the graph.

At this point, it must be noted that it was necessary to extend the range of integration, insofar as the effects of ionization and elastic processes were concerned, to 40 eV for the higher values of  $E/N$ . This was necessary to obtain a meaningful approximation to the ionization rate integral, because the tail of the distribution function between 20 eV and 30 to 35 eV gave a nonnegligible contribution to the rate for higher values of  $E/N$ . For the case of ac fields, the problem of the high energy tail of the distribution function does not develop until fields considerably above breakdown are encountered. Also, it was noted that the  $f_1(u)$  term of the expansion became a large fraction of  $f_0$  for  $E/N$  greater than  $4 \times 10^{-15} \text{ V-cm}^2$ .

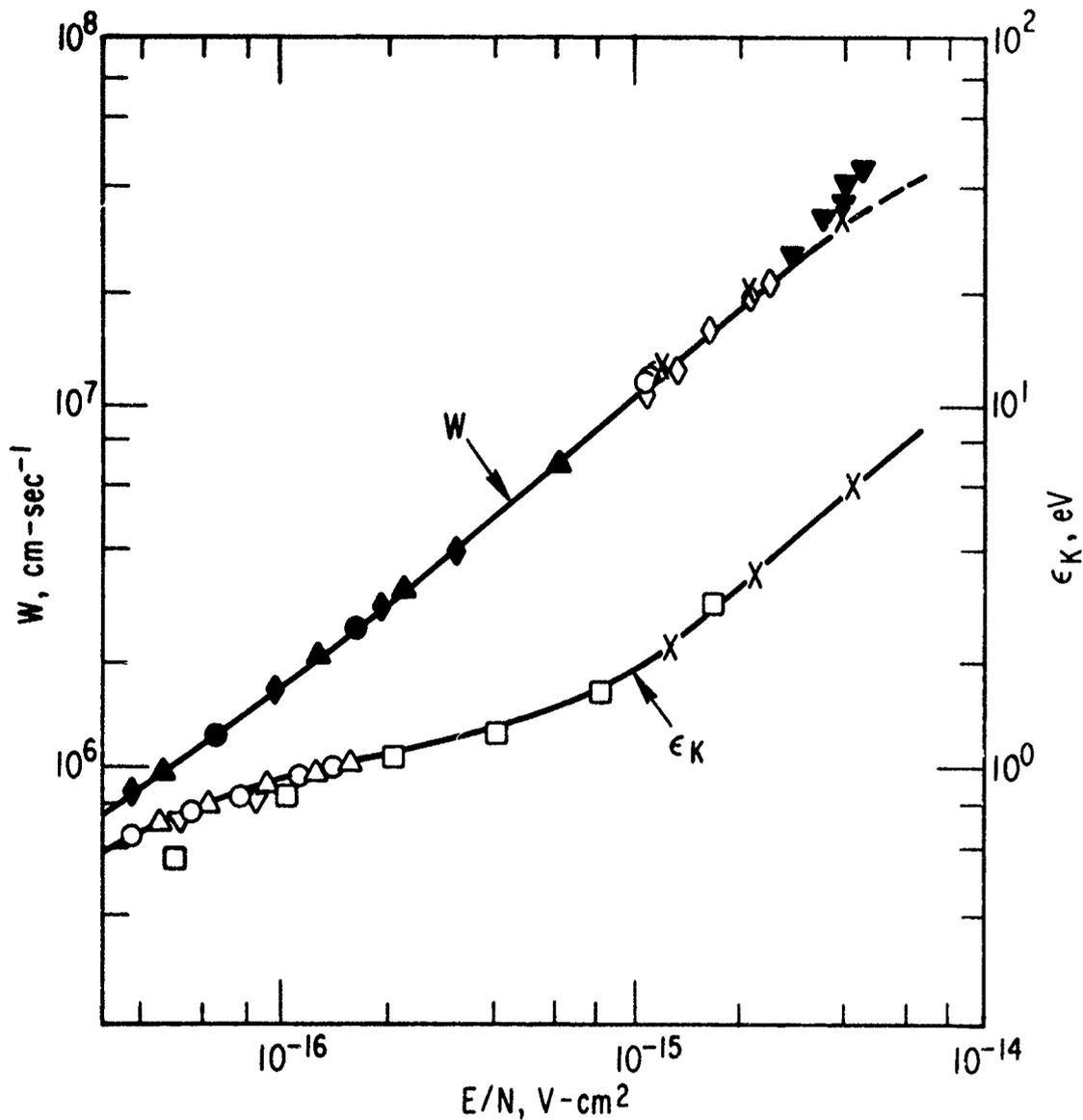


Fig.1. Comparison of drift velocity and Phelps' characteristic energy for  $N_2$  in a dc field in the  $E/N$  range of interest in breakdown studies. [  $\times$  's represent the results of typical calculations performed in this study; other symbols represent data from Ref. 6. Illustration is from Phelps (Ref.6, Fig.4), courtesy of the American Institute of Physics.]

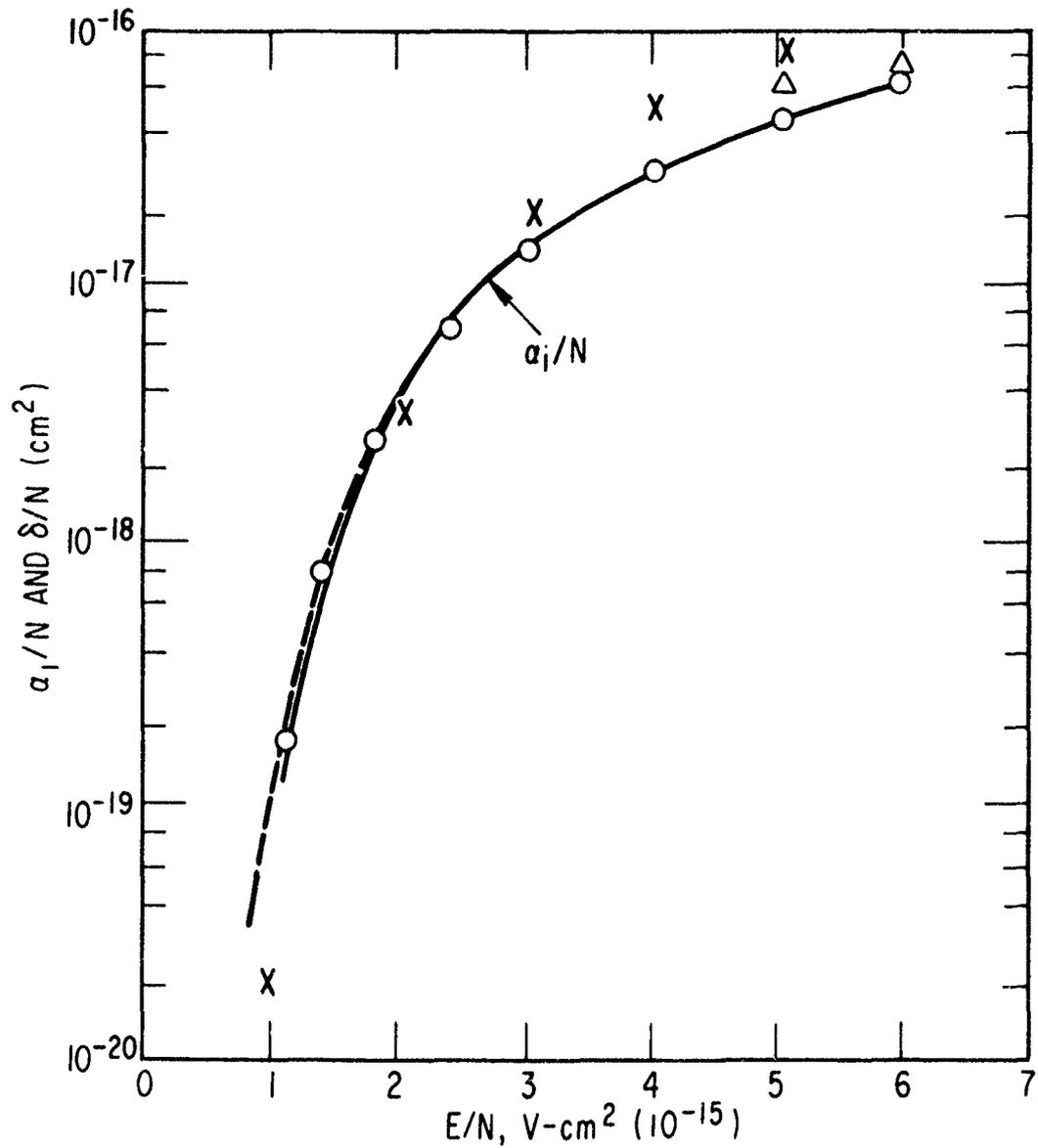


Fig.2. Comparison of the first Townsend ionization coefficient for  $N_2$  in a dc field in the  $E/N$  range of interest in breakdown studies. [ 'x' 's represent the results of typical calculations performed in this study; other symbols represent data from Ref. 6. Illustration is from Phelps (Ref. 6, Fig.7), courtesy of the American Institute of Physics.]

Figure 1 shows the reported values of Phelps' characteristic energies  $\epsilon_K$  and the drift velocity  $w$  with the calibration run values shown as X's. Figure 2 shows the agreement of the Townsend ionization coefficient; the computational results are shown as X's. The disagreement in this figure becomes appreciable for values of  $E/N > 3 \times 10^{-15} \text{ V-cm}^2$ . At this point, the first order expansion term is about 0.75 of the zeroth order term, so the spherical distribution function approximation is far from valid. Also, about 10% of the electron energy loss is through ionization, which means that new electrons are being generated at a non-negligible rate. These conditions are well above breakdown and, hence, will not effect the eventual purpose of the program.

A further comparison of the difference between Phelps' solution and the present one is provided at  $E/N = 3 \times 10^{-15} \text{ V-cm}^2$  where he shows a value of  $\epsilon_K$  is 4.6 eV and the present result is 4.3 eV. This difference may come from the ionization process treatment discussed in Section IV.

Further close agreement is found with the average energy defined as 1.5 times the diffusion coefficient divided by the mobility as shown in Brown (Ref. 10). This particular plot points out the fallacy in the assumption by MacDonald (Ref. 3, p. 176) that the average electron energy is linear in  $E/p$ , where  $p$  is the pressure, when the experimental data show (Ref. 10) that the variation is logarithmic in  $E/p$ .

## VII. HIGH-PRESSURE MICROWAVE EXPERIMENTAL COMPARISON

For a driving frequency of 9.375 GHz in air at 100 torr, the electron collision frequency is much less than the driving frequency, and the "effective field" frequently used to correlate experimental data is practically the same as the applied field. This fact was utilized to provide a further check of the program's output by comparison with experimental plots of net ionization frequency vs "effective" electric field strength.

Thompson has verified the ionization rate data obtained by other researchers (Ref. 11). Thompson's (Ref. 12) results are presented in Fig. 3 with the calculated results obtained from the computer program. The agreement is seen to be qualitatively and quantitatively correct and falls well within the experimental error bars.

For the 9.375 GHz field necessary to breakdown air at 100 torr, the value calculated by the program is between 3000 and 3500 V-cm. This value lies on the curve given by MacDonald (Ref. 3, p. 165).

The mobility calculated at breakdown is  $1.44 \times 10^6$  V-cm<sup>2</sup> - sec, which may be compared with a result from an analysis attributed to Brown (Ref. 3, p. 172), which gives a value of  $1.25 \times 10^6$  V-cm<sup>2</sup>-sec. This is a disagreement of less than 15% with the experimental mobility.

Agreement with low-pressure "effective field" results is not forthcoming because the "effective field" concept is not valid because of the strong variation of collision frequency with electric field strength as may be seen in Fig. 4. It is not too surprising to see that the collision frequency exhibits a dependence on electric field strength and frequency as well as pressure. An examination of Eq. (2) for the time-dependent case shows that the differential equation cannot transform in such a way as to exhibit the "effective field" results unless certain conditions are met. For the net  $(\nu_1 - \nu_a)/p$  to be invariant with

$$E/p \left[ 1 + \left( \frac{\omega}{\nu_c} \right)^2 \right]^{1/2}$$

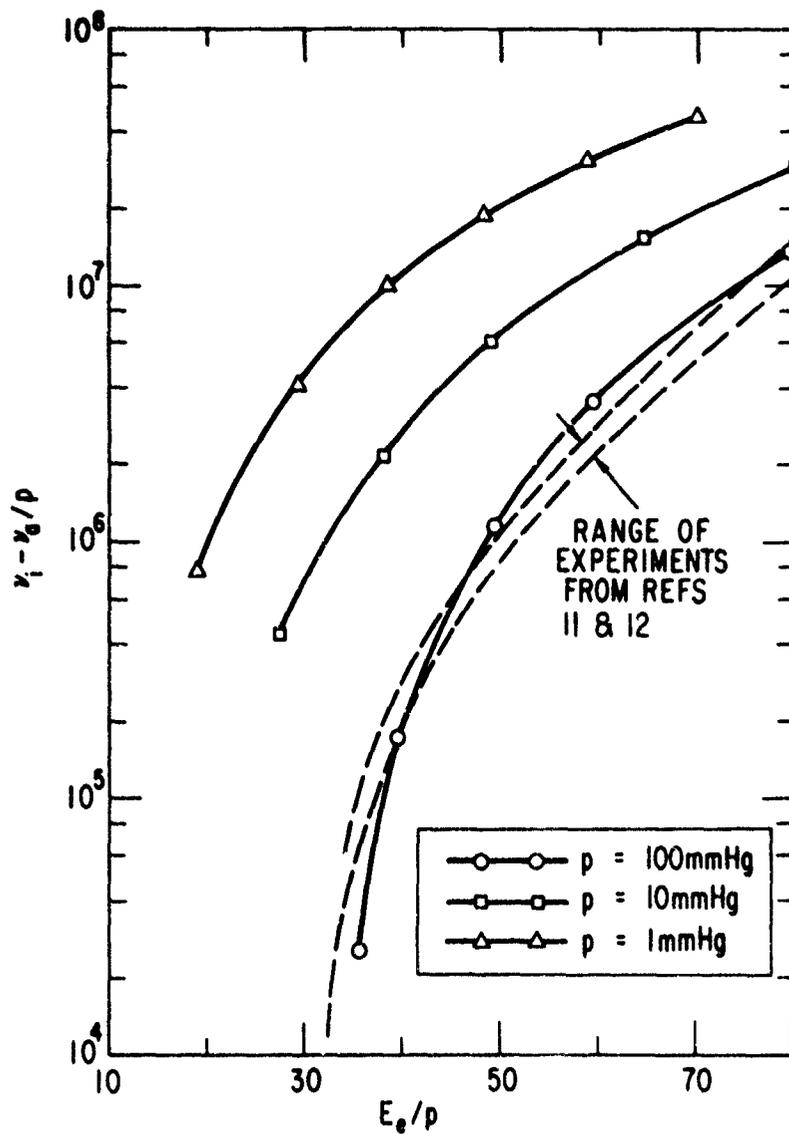


Fig.3. Net ionization frequency for air calculated with an ac driving field of 9.4 kMc in comparison with experimental values from Refs. 11 and 12, plotted as a function of effective field for various pressures. [Illustration is from Epstein and Lenander (Ref. 13, Fig. 3)]

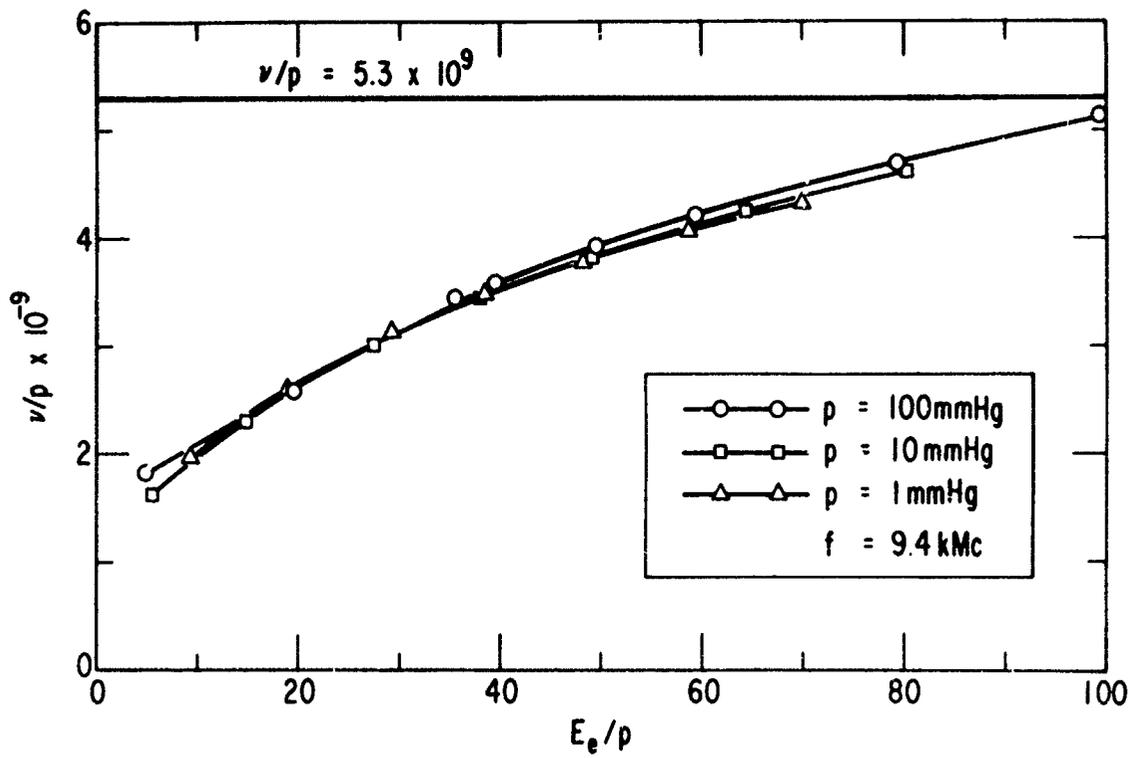


Fig. 4. Average total collision frequencies as a function of effective field for various pressures, shown with the frequently suggested value of  $5.3 \times 10^9$ . [Illustration is from Lenander (Ref.5).]

the "effective field" divided by pressure must be a constant. This is required so that the electron distribution function shape will be independent of pressure and produce the same collision frequency integral. This, in turn, is obtainable, consistent with the assumption that  $\nu_c$  varies linearly with pressure, only if the energy-dependent total collision frequency is replaced by a constant. If  $\nu_c$  is energy dependent, as it must be, the nonlinearity of Eq. (2) emphasizes the error inherent in the "effective field" approach.

From these comparisons, it appears that the calculated observable quantities for 9.374 GHz excitation at  $p = 100$  torr agree quite well with experimental values.

## VIII. SUMMATION AND CONCLUSIONS

The NBS computer program for solution of the Boltzmann equation using a multicross-section model for air was converted and updated for use at Aerospace for prediction of microwave breakdown. This involved a reevaluation of the basic theory, a more physical treatment of the ionization products, and a determination of the most reliable and representative cross sections in air.

The program was tested for determination of its ability to solve the Boltzmann equation exactly for the Maxwell solution. The data pack of cross sections was verified as being representative of air by calculation of the observable quantities: electron mobility, diffusion coefficient, ionization coefficient, and net ionization frequency. Good agreement was obtained with values already known from experiment.

On the basis of the calculated test results, it is felt that the program and the data pack will produce meaningful predictions of microwave breakdown in air.

## APPENDIX

### The Computer Program

The program produces an inward integration of Eq. (2) utilizing a data table of cross sections defined on each 0.10 eV from 0 to 20.0. The data table is in the form of a binary tape, which has the cross-section thresholds as the first record and the 36 cross sections (some are zero dummies) as the next 36 records.

Data input directly to the program consists of the density fractions of  $O_2$ ,  $O$ , and  $N_2$ ; amu masses of  $O_2$ ,  $O$ , and  $N_2$  (must not be zero); gas temperature,  $^{\circ}K$ ; pressure, torr; rms electric field strength, V-cm; driving frequency, cps; magnetic field perpendicular to the electric field, gauss; and the maximum energy for the integration, eV ( $\leq 20$ eV). The units of the integration are a mixture of esu, cgs, and eV.

The energy step of the integration is the energy range divided by 2000. As the inward integration proceeds, the necessary cross-section values are obtained by linear interpolation of the data table values at the nearest 0.1 eV points.

As the inward integration proceeds, the distribution function value is tested to prevent overflow, which can result from too large an energy range, and the function derivative is tested to find the energy at which the Lorentz term is the largest. Step by step, the observables or moments of the distribution function are calculated. The proper normalization is supplied at the end of the integration.

The output quantities are: the gas constituent densities; gas temperature; total gas pressure; energy increment for the integration step; the driving electric field and its frequency; the magnetic field strength; the effective field based on the calculated total collision frequency; the average electron energy; average electron speed; total collision frequency; conductivities parallel and perpendicular to the electric field and the Hall magnetic conductivities per electron; diffusion coefficient; drift velocity; Phelps' characteristic energy defined as the diffusion coefficient divided by the drift velocity, expressed in eV; mean free path; average interparticle distance; a table of the rate constants for

each of the cross sections considered and the amount of electron energy loss to each;  $O_2$  radiative attachment rate;  $O_2$  dissociative attachment rate; total ionization rate; the normalization factor; the largest ratio of the Lorentz term to the zeroth order term and the energy at which it occurs; and a listing of this distribution function at each tenth point of the integration range on the corresponding energy. All the above quantities are written out in cgs-esu or are clearly labeled.

When the calculations for one case are complete, the program looks for a new set of input data before terminating. No provisions are made within the program that prevent improper solutions or indefinite numbers. It is assumed that the data input to the program is correct and of a reasonable nature such that problems of that type will not arise.

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