# MONTE CARLO INVESTIGATIONS OF NON-EQUILIBRIUM EFFECTS AT HIGH VALUES OF E/p IN SWARM EXPERIMENTS IN HYDROGEN

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#### Abstract

The results of a Monte Carlo computer simulation of the properties of electrons in a gas at pressure p subjected to a constant electric field E are presented for  $E/p = 350 \text{ V cm}^{-1} \text{ torr}^{-1}$  in hydrogen. Evidence is provided that the spatial growth of ionization is essentially non-equilibrium in these circumstances and that the general form of the predicted growth of currents is consistent with experiment. Analysis of the theoretical data leads to an effective value of the primary ionization coefficient  $\alpha/p$  in satisfactory agreement with experiment.

#### I. INTRODUCTION

Many discrepancies persist in the literature on ionization coefficients (Dutton 1967) despite a considerable experimental effort to resolve them, and it can hardly be claimed that our understanding of the problem is satisfactory. The complexity of the situation increases with increasing E/p, and from the recent thin-film investigations of Haydon and Stock (1966) it seems clear that many of the difficulties arise through inadequate appreciation of the influence of instrumental factors on the non-equilibrium ionization growth associated with the early stage of the avalanche development. In that investigation, analysis of the ionization data was carried out assuming the well-known Townsend equation

$$I = I_0 \exp \alpha (d - d_0) / [1 - (\omega/\alpha) \{ \exp \alpha (d - d_0) - 1 \} ],$$
(1)

where  $I_0$  is the initial photoelectric current from the cathode,  $\alpha$  and  $\omega/\alpha$  are the primary and secondary ionization coefficients, and the quantity  $d_0$  is a distance introduced to take account of non-equilibrium effects at very small separations. However, it is not clear that there is any real justification for using this "equilibrium" equation at high values of E/p, where it has not yet been established that a transition to a true equilibrium situation is in fact achieved. This equilibrium could be inhibited for instance by the efficient secondary ionization mechanisms leading to a breakdown event at values of the parameter pd too low for equilibrium to have been reached. Clearly the initial growth must become increasingly non-equilibrium in character, the larger the difference between the mean energy ( $\sim 0.5 \text{ eV}$ ) of the initial group of photoelectrons and the high mean energies ( $\geq 30 \text{ eV}$ ) achieved at high values of E/p.

One hopeful development, which forms the basis of the present paper, lies in the use of Monte Carlo computer techniques to predict the spatial growth of current.

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This provides the opportunity, given reliable data for electron-molecule collision cross sections, to compute ionization currents as a function of pd for comparison directly with experiment and for analysis by procedures presently used to obtain information about the fundamental primary  $(\alpha/p)$  and secondary  $(\omega/\alpha)$  ionization coefficients from experimental data. For the large values of pd required to investigate low values of E/p, a very large number of collisions is necessary before an electron and all its progeny are collected and recorded as an avalanche of electron ionization. However, for the low values of pd used at high values of E/p, the number of collisions is considerably reduced and initially our studies have been confined to this region.

Simplifying assumptions were made in the early Monte Carlo work of this nature as, for example, by Itoh and Musha (1960), who assumed isotropic scattering for all collisions and ignored the scattered electrons formed by ionization in the gas. Thomas and Thomas (1969), however, simulated entire avalanches and introduced anisotropy into the electron scattering as suggested by Fleming (1966). They studied electron ionization in neon and adjusted the cross sections for electron-atom collisions to achieve agreement between their calculated values of  $\alpha/p$  and those obtained experimentally.

In the present investigation, however, we are particularly concerned to establish the nature of any spatial variation of the ionizing properties of the electrons and to assess critically the validity or otherwise of applying the equilibrium ionization growth equations to obtain fundamental ionization coefficients.

The principle of the method is to consider the collision interactions with neutral gas particles made by a single electron of specified energy during its progress across the gap, until its final collection at the anode boundary walls of a plane-parallel electrode configuration. Given knowledge of the probabilities for the various events, random number techniques are used to determine the nature and number of collision processes. The single electron treatment is extended to include a group of electrons typical of those generated in experiment by irradiation of the cathode surface with ultraviolet light.

It is shown from such calculations, in which non-isotropic scattering is considered, that the general form of the predicted growth of current is in accord with that observed in experiment, and furthermore that non-equilibrium effects must be considered when analysing experimental data.

These non-equilibrium effects occur at small gap separations and large values of E/p and have been the subject of special experimental investigation in the present study. Modifications to the ionization chamber used in an earlier investigation (Haydon and Stock 1966) have allowed deliberate perturbations of the electric field conditions in these early stages of ionization growth, and, when this ionization has been analysed using the Gosseries technique, characteristic curvatures in the reciprocal ionization current plots have provided a better insight into the non-equilibrium phenomena. These curvatures have been predicted by the Monte Carlo computations of the ionization growth, and with a clearer understanding of the non-equilibrium effects a considerable amount of reliable data has now been accumulated at  $E/p = 350 \text{ V cm}^{-1} \text{ torr}^{-1}$  in hydrogen. For this reason the detailed treatment of the Monte Carlo calculations given in Section IV below has been applied to this particular situation. Since comparison of the Monte Carlo predictions of the non-equilibrium

phenomena with experiment are of special interest, it is first necessary to examine in more detail the experimental method, analytical procedures, and the various effects observed in the reciprocal Gosseries plots which would be interpreted as nonequilibrium effects.

### II. EXPERIMENTAL METHOD AND ANALYTICAL PROCEDURES

In considering the steady-state equilibrium growth of ionization, the philosophy underlying all the experimental investigations has been essentially the same and concerned primarily with obtaining I versus pd curves for constant values of E/p. Analysis of this information has been based on equation (1) in which there are four unknowns, namely  $I_0$ ,  $\alpha$ ,  $\omega/\alpha$ , and  $d_0$ . Various procedures are available for obtaining these quantities including a "three-point" method originally used by Townsend and MacCallum (1928). In this method the currents  $I_1$ ,  $I_2$ , and  $I_3$  are measured at distances  $d_1$ ,  $d_2$ , and  $d_3$  and by then setting  $d_2-d_1=d_3-d_2=\Delta d$  equation (1) transforms to

$$\exp\left(\frac{\alpha\,\Delta(pd)}{p}\right) = \frac{I_3\,I_2 - I_1}{I_1\,I_3 - I_2}.\tag{2}$$

This equation or a generalized form of it has been used by Jones and Llewellyn Jones (1958), Davies, Llewellyn Jones, and Morgan (1962), Chanin and Rork (1963), and others. Another method, due to Gosseries (1939), is based on plots of reciprocals  $Y_d$  of currents measured at distances d and  $d + \Delta d$ . Since equation (1) transforms to

$$Y_d = Y_{d+Ad} \exp(\alpha \Delta d) + Q\{\exp(\alpha \Delta d) - 1\}, \qquad (3)$$

the slope of the graph of  $Y_d$  versus  $Y_{d+\Delta d}$  gives a value for  $\alpha/p$ . This method extends the three-point technique to include all measured values, and has been used in our studies at Armidale (Haydon and Robertson 1961; Haydon and Stock 1966). More recently (Golden, Nakano, and Fisher 1965; Lake-Thomas, personal communication), several computer programs have been developed which analyse experimental I, dcurves using a least-squares error iterative procedure to derive  $\alpha$ ,  $\omega/\alpha$ ,  $I_0$ , and  $d_0$ .

A further method used at low E/p where equilibrium conditions are well satisfied and  $\omega/\alpha$  is  $\ll 1$  obtains  $\alpha/p$  from a semilog plot of I versus d at small distances. It is not valid in the experimental situations we are presently discussing.

Although the various analytical procedures used at high E/p have been criticised for specific deficiencies, they are nevertheless all basically identical. In view of this and the superficial simplicity of the experiment itself, it seems very surprising that such large discrepancies as shown in Table 1 should persist in the literature.

These discrepancies cannot be attributed entirely to the analytical procedures that have been used. For example, some data obtained for hydrogen at  $E/p = 350 \text{ V cm}^{-1} \text{ torr}^{-1}$  yielded identical values for the ionization coefficients whether analysed by the Gosseries technique or by elaborate computer programs developed at two other laboratories (Golden, Nakano, and Fisher 1965; Lake-Thomas, personal communication). For this reason the Gosseries technique has continued to be used to analyse data obtained in our laboratories, and an explanation for the discrepancies is believed to be associated with the basic I, d data. Although experimental evidence to support this has already been published (Haydon and Stock 1966), no detailed theoretical study has so far appeared. Before considering the results of the present Monte Carlo calculations, it seems important to stress one assumption of the growth equation (1) which may not be adequately appreciated. This concerns the  $d_0$  concept.

E/p at 0°C (V cm <sup>-1</sup> torr <sup>-1</sup> )	Rose (1956)	Jones and Llewellyn Jones (1958)	Davies and Milne (1959)	Haydon and Robertson (1961)	Chanin and Rork (1963)	Golden, Nakano, and Fisher (1965)	Haydon and Stock (1966)
50	0.315	0.315	0.317	0.315	0.310	0.315	0.315
300	$3 \cdot 21$	$2 \cdot 40$	$2 \cdot 97$	$2 \cdot 55$	$3 \cdot 57$	$3 \cdot 21$	$2 \cdot 55$
350	$3 \cdot 45$	$2 \cdot 52$	$3 \cdot 09$	$2 \cdot 56$	3.68	$3 \cdot 50$	$2 \cdot 55$

TABLE 1												
SUMMARY	OF	EXPERIMENTAL	$\alpha/p$	VALUES	IN	HYDROGEN						

In the model of Townsend and MacCallum (1928), the actual non-equilibrium distance  $d'_0$  ( $\neq d_0$ ) is replaced by  $d_0$ , it being assumed by so doing that we can regard  $\alpha = 0$  in the region d = 0 to  $d_0$  and equal to the constant equilibrium value  $\alpha$  in the interval  $d > d_0$ . Clearly we must be especially careful not to use equation (1) when analysing ionization currents obtained in the non-equilibrium region d = 0 to  $d'_0$  ( $> d_0$ ). For this reason it becomes necessary to establish some criterion for identifying these non-equilibrium conditions which include not only the fundamental equilibrium problem but also the instrumentally induced non-equilibrium effects. Only by eliminating the instrumental effects can we hope to establish whether an equilibrium, in which  $\alpha$  and  $\omega/\alpha$  are constant independent of distance, is in fact achieved.

Whilst the preliminary measurements reported by Haydon and Stock (1966) using thin gold film techniques represented a considerable improvement in controlling the instrumental effects, some uncertainties remained about the reliability of observations made at very small gap separations. Furthermore, photons generated in the avalanches could leave the uniform field region of the ionization gap and lead to electron amplification not strictly representative of the ideal infinite plane-parallel electrode geometry for which equation (1) should be valid.

For this reason a new ionization chamber using split electrode geometry of large dimensions (total plane electrode diam.  $8 \cdot 26$  cm; central disk diam.  $3 \cdot 02$  cm) and thin-film techniques was constructed. The electrodes were parallel to within 0.003 mm over the central disk diameter and the gap separations, continuously variable from 0-3 cm, were known to better than 0.01 mm. Further details of the experimental arrangements will be given elsewhere (Folkard and Haydon, to be published). The measurements with which the Monte Carlo calculations were compared, have been carried out in this new apparatus and represent the most reliable set of data we have so far been able to record.

Qualitatively, it could be reasoned that, at any distance d = x,  $\alpha(x)$  should be an increasing function of x until equilibrium is established. However, if electrons gain energy and "run away", conditions develop to the stage where the ionization probability exceeds the maximum value and begins to fall, when we might anticipate  $\alpha(x)$  being a decreasing function of x. One analysis (Chanin and Rork 1963) provides some evidence for this latter situation. Although we would expect this at very large values of E/p, our present measurements do not confirm this interpretation for the special case  $E/p = 350 \text{ V cm}^{-1} \text{ torr}^{-1}$  in hydrogen.



Fig. 1.—Modified ionization chamber for the study of current growth under perturbed non-equilibrium conditions.

### III. EFFECT OF NON-EQUILIBRIUM ON GOSSERIES ANALYSIS

Previous work showed that given unfavourable electrode geometry and instrumental non-equilibrium effects, reliable and consistent values for the ionization coefficients could only be obtained by confining analysis to measurements made at large distances corresponding to applied voltages  $\geq 70-100$  V. This is a consequence of the fact that  $\alpha$  is a function of position at small electrode separations and was demonstrated quite clearly in the present investigations when some controlled perturbation of the non-equilibrium region was introduced. This was achieved by incorporating a subsidiary gap, separated from the main gap by a wire mesh, in a modified version of the ionization chamber used by Haydon and Stock (see Fig. 1). Here, electrons generated at A by the thin-film technique move across the subsidiary gap under conditions determined by the value of E'/p ( $\leq E/p$ ) and enter the main gap through the wire mesh B. Although this wire mesh introduces field distortions in the main gap, it is possible nevertheless to study in the main gap the general characteristics of the ionization growth as it varies due to perturbations created by E'/p varying from 0 to E/p in the subsidiary gap.

In previous investigations, the downcurving on nonlinear Gosseries plots at small d was interpreted in terms of a true non-equilibrium in which electrons were required to travel a distance  $d'_0$  before acquiring the mean energy appropriate to the applied E/p. Any upcurving at small separations was considered to be due to field nonuniformities caused by the anode holes.

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Figure 2, showing Gosseries plots at  $E/p = 350 \text{ V cm}^{-1} \text{ torr}^{-1}$ , confirms this broad interpretation. More specifically, for  $E/p = 350 \text{ V cm}^{-1} \text{ torr}^{-1}$  with E'/p = 0, the plot is linear for V > 70 V, while for V < 70 V downcurving takes place, i.e. on our previous interpretation, the non-equilibrium effect is dominant in this region. However, by contrast, the plot for E'/p = 350 can be linear down to 35 V while pronounced upcurving is evident for V < 35 V. Similar behaviour is observed for  $E/p = 100 \text{ V cm}^{-1} \text{ torr}^{-1}$ , but here the subsidiary gap at E'/p = 100 allows the electrons to settle into equilibrium after just 25 V. This extension of the range of linearity to lower values of V can be understood if the function of the subsidiary discharge gap is merely to enable the electrons to settle more rapidly into equilibrium with the applied field in the main gap. The upcurving of the Gosseries plots always present at the smallest separations is due to the field nonuniformities introduced by the mesh.



Fig. 2.—Gosseries plots for  $E/p = 350 \text{ V cm}^{-1} \text{ torr}^{-1}$  and p = 0.62 torr in hydrogen for two values of  $\Delta d$  and E'/p = 0 and 350 V cm<sup>-1</sup> torr<sup>-1</sup>.

Two further points should be stressed. Firstly, in plotting reciprocal currents in the Gosseries analysis, large errors can intrude at small gap separations corresponding to large values of  $Y_d$  and  $Y_{d+\Delta d}$ . Nevertheless, the behaviour shown in Figure 2 is characteristic of every set of measurements and represents a reproducible phenomenon. Secondly, the ionization coefficient  $\alpha$  is obtained unambiguously from the slope of the appropriate Gosseries plot, provided only that the other parameters  $I_0$ ,  $d_0$ , and  $\omega/\alpha$  remain constant during the course of the experiment. For an idealized situation in which we have no secondary ionization processes contributing to the growth of current, an extrapolation of the linear Gosseries plot would pass through the origin rather than intercept the  $Y_d$  axis at a positive value. The slope of the linear plot would still, however, be the same and yield the same value for the primary ionization coefficient  $\alpha/p$ . This means that as a first stage in the complex computations by the Monte Carlo technique, a useful insight into the problem should be possible by considering only the primary electron-molecule collision interactions. This has the advantage that it allows a consideration of the ionization growth at electrode separations much larger than are possible experimentally, where secondary processes may yield a breakdown event before the natural equilibrium has been achieved.

## IV. MONTE CARLO METHOD

For convenience in applying the results to several different situations, the present calculations were carried out in three stages. Firstly, the distances moved on average by an electron of specified energy both in the field direction and directly against the field were computed. Secondly, the actual distance moved by such an electron was determined by considering the distribution of paths about the average value. Thirdly, the nature of the collision that terminates each free path was determined from a knowledge of the probabilities for the various collision interactions.

In the first stage, properties such as the distance moved between collisions with gas molecules, the component of this distance parallel to the applied field, and the time interval between collisions were determined for many individual electrons of the same initial energy. These properties were derived from the equations of motion for each electron in a steady electric field at unit gas pressure, and the behaviour of a typical electron of this initial energy was then represented by the average of each of the properties of all the individual electrons. Thermal motions of the gas molecules were neglected, and the range of electron energies considered extended to  $\sim 200 \text{ eV}$ . At high E/p where the electrons have large mean energies, scattering of the electron at a collision interaction becomes highly directional. The asymmetry thus introduced into the scattering process assumes increasing importance as the electron energy increases and, in this investigation, was taken into account by a weighting factor dependent on the experimental scattering data of Bullard and Massey (1931) and Webb (1935). At high electron energies most electrons, after collision, move through only a small angle  $\theta$  with respect to their original direction and reliable data for small-angle scattering is therefore needed. In the absence of such experimental data an extrapolation of polar plots of  $I(\theta)$  against  $\theta$  (where  $I(\theta) d\Omega$  is the relative number of electrons scattered after collision into a solid angle  $d\Omega = 2\pi \sin\theta \,d\theta$  was used to estimate the values of  $I(\theta)$  required to determine the weighting factors  $P(\theta)$  at small  $\theta$ . This weighting factor was taken to be

$$P( heta) = \int_0^ heta I( heta) \sin heta \, \mathrm{d} heta \, \Big/ \, \int_0^\pi I( heta) \sin heta \, \mathrm{d} heta \,, \qquad 0 \leqslant P( heta) \leqslant 1 \,,$$

and since  $\sin \theta \to 0$  for  $\theta \to 0$  or  $\theta \to \pi$ ,  $I(\theta) \sin \theta$  is insensitive to any errors introduced by the above extrapolation process. For this reason the weighting factor  $P(\theta)$  is also insensitive to such an extrapolation. Values of  $P(\theta)$  as a function of  $\theta$  calculated in this way enabled the angle  $\theta$ , which determined the direction of electron motion with respect to the electric field, to be determined after equating a random number to  $P(\theta)$ .

It was assumed that the scattering data for a specific electron energy adequately represented the situation for groups of electrons with energies ranging on either side of the specified energy. Thus, as a simplifying approximation the scattering characteristics for electrons with energies between 2–6, 6–15, 15–40, and 40–200 eV were assumed to be the same as those given by data for 4, 10, 30, and 50 eV electrons respectively. Electrons with energies between 0–2 eV were assumed to be scattered

isotropically. For convenience in later stages of the program, the electrons were also separated into two discrete groups, depending on whether (1)  $0 \leq \theta \leq \frac{1}{2}\pi$  ("forward" event) or (2)  $\frac{1}{2}\pi < \theta \leq \pi$  ("backward" event). A single electron of energy U then moved a distance step  $\Delta L$  in this direction  $\theta$ , where (1)  $\Delta L$  was less than 10% of the mean free path  $L = (NQ_{\text{tot}})^{-1}$  and (2) the energy gained from the field over this distance step was less than 10% of the electron energy at the beginning of the step. These conditions were imposed to ensure that electron properties would not alter significantly over the step  $\Delta L$ , since the actual curved trajectory of the electron is here simply replaced by a series of such linear elements  $\Delta L$ . The probability of collision within the step  $\Delta L$  was

$$1-\exp(-\Delta L/L)$$
,

and comparison of this value with a normalized random number determined whether a collision had in fact occurred in this distance step  $\Delta L$ . If no collision had taken place then it was necessary to correct the trajectory to correspond to the curved path which a real electron would have taken. The new electron direction and velocity were found at the end of  $\Delta L$  by first calculating the additional momentum and energy acquired by the electron from the field E during the time taken to traverse the distance  $\Delta L$ and then solving the corresponding conservation equations. After the new direction had been determined, the electron continued to traverse another step  $\Delta L$  appropriate to the new energy it had acquired at the end of the previous step. This step process continued until the free path was terminated by a collision.

Since the actual collision will not necessarily occur at the end of an element  $\Delta L$ , the fraction of the final step at which the collision takes place was determined by a random number procedure. The sum of the distances  $\Delta X$ , where  $\Delta X$  is the component in the field direction of each element or fraction of element  $\Delta L$ , and  $\Delta L$  is oriented at an angle  $\theta$  to the field, was recorded for this electron. A new electron with the same initial energy but different initial direction was then generated, and its properties upon collision determined. This process was repeated for many electrons, with the initial orientation  $\theta$  determined in each case by comparison of individual random numbers with  $P(\theta)$ . The average values for the distance components moved by an electron both in the field direction and against the field direction,  $L_1$  and  $L_2$ respectively, were then determined. It must be appreciated that the distances  $L_1$ and  $L_2$  (shown in Fig. 3, curve B, as a function of the initial energy of the electrons) are the average values for the components  $(\sum \Delta X)$  and as such have only two orientations with respect to the electric field, that is, forward ( $\theta = 0^{\circ}$ ) and backward  $(\theta = 180^{\circ})$  respectively. For comparison the results of similar computations made on the basis of isotropic scattering are shown in Figure 3, curve A.

Having calculated the average distances travelled by a typical electron of specified initial energy, it was necessary in the second stage to retrieve information about the actual distances travelled by individual electrons in the forward and backward directions. A rigorous approach would determine, from the results of the first stage, the distribution of actual distances about the mean value for each group of electrons selected in the range 0–200 eV. If in fact these distributions are functions of energy, then some interpolation procedure would be necessary to obtain the actual distribution of distances appropriate to each electron energy. Even though this

information could be obtained from the first stage, its application to the calculations required in the third stage below becomes very complex, and to obtain Monte Carlo predictions of ionization growth over the required wide range of values of E/p would involve excessive computer storage facilities. The consequences of not following this rigorous procedure are under investigation, but for the present purposes it is sufficient to retrieve the actual distances moved between collisions by assuming the usual exponential behaviour for the distribution of paths about the mean values  $L_1$  and  $L_2$ .



Fig. 3.—Comparison of Monte Carlo calculations of mean path lengths  $L_1$  and  $L_2$ as a function of initial electron energy U for:

A, isotropic scattering

B, anisotropic scattering

Knowledge of the actual distances moved in the forward and backward directions then permitted a determination of the nature of the collision interaction which terminated the actual free path. This formed the third stage of the calculations, in which the anisotropy of the collision interaction was taken into account in the following way:

The fraction of scattering events which resulted in deflection of an electron through an angle  $\theta$  with respect to its initial direction, could be determined from the  $P(\theta)$  values calculated for electrons of each energy group. In this way the proportion of electrons scattered through  $0 < \theta \leq \frac{1}{2}\pi$  and the corresponding proportion scattered through  $\frac{1}{2}\pi < \theta \leq \pi$  could be determined.

Since the energy gained from the electric field determines the transport properties, we are primarily interested in the characteristics of the scattering events about the field direction, and the information obtained above should be made more relevant by taking into account the angle between the direction of the electron immediately before collision and the direction of the electric field itself. In practice this would involve a number of complex computations and in view of the uncertainties about some of the scattering data that are available, the computing time and effort that would be required were not considered justified. For the present purposes therefore, we have neglected this correction. Nevertheless, a rough estimate of the probable influence of such an assumption can be made on the basis of information recorded in the first stage, which shows that the difference between the two directions for electrons of energy  $\geq 20 \text{ eV}$ , possessing the average properties, is certainly less than 18°. This means that the correction to be applied involves the difference in the probability of scattering between  $72^{\circ}-90^{\circ}$  and  $90^{\circ}-108^{\circ}$ . The value of this difference was estimated from available data for electrons of energy  $\geq 20 \text{ eV}$  to be  $\sim 1\%$ , so that on this basis we have essentially considered 1% too many electrons to be travelling in the forward direction. This should have the effect of yielding ionization currents and coefficients that are too high and one would not expect complete agreement between the values of ionization parameters computed on this assumption and those observed experimentally. Once again, however, the broad characteristics of the electron behaviour should not be greatly altered.

With this information on the fraction of forward and backward events, random number techniques were then applied to determine whether a specific electron would move towards the anode ( $\theta = 0^{\circ}$ ) or towards the cathode ( $\theta = 180^{\circ}$ ), after its previous collision.

For the actual computation of ionization currents, the procedure reduces to considering a single electron of energy 0.5 eV generated at the cathode, and moving towards the anode parallel to the electric field. The distance step moved by the electron was based on the distribution of forward paths about  $L_1$  and, whilst travelling this distance, the electron gained energy from the applied field. At the end of this distance step, a collision would occur. The type of collision (elastic, vibration, dissociation, photon excitation, and ionization were considered) depended on the electron energy at the end of the step, and was determined by comparison of a random number with the probabilities for the various processes. These probabilities were obtained from cross section data based on the determinations of Tate and Smith (1932) and Engelhardt and Phelps (1963).

Once the type of collision had been recorded, a random number determined whether the subsequent electron motion was in the initial direction  $\theta = 0$  or whether a backward scattering event had taken place. The magnitude of the distance step moved before the next collision was calculated, and the type of collision which terminated the step was determined as for the first collision. After each step moved in the gas, a test was made to ensure that the electron was still in the ionization region, i.e. that it had neither been recaptured at the cathode nor collected at the anode. This process was continued until the electron under consideration reached the anode.

When an ionizing event occurred and a new electron was formed, the available energy was assumed to be shared randomly between the scattered and ejected electrons, and relevant data such as energy and position of the ejected electron were stored. The initial electron continued to be traced during its progress across the gap (storing data on all its progeny) until it was collected at the anode. The stored data for each additional electron resulting from an ionizing collision were then retrieved in turn, and these electrons (and their progeny) traced to the anode. This process was repeated until the entire avalanche generated by the single initial electron of energy 0.5 eV had been collected. When an entire avalanche had been recorded, the calculations were repeated for another initial electron of this energy and so another avalanche was traced. The program allowed printout of the numbers of initial and collected electrons, the numbers of the various types of collisions and the amount of energy lost in each process, the mean energy of electrons on reaching the anode, and the distribution of electron energies about the mean value.

### V. SUMMARY OF MONTE CARLO CALCULATIONS AND COMPARISON WITH EXPERIMENT

Since the primary interest in the present investigation was to establish the nature of any spatial variations of the properties of the electrons, we consider specifically the evidence for any non-equilibrium in (a) the mean energy and (b) the ionization coefficient  $\alpha/p$  as revealed by the Monte Carlo method. The results are appropriate for hydrogen at  $E/p = 350 \text{ V cm}^{-1} \text{ torr}^{-1}$ .



Fig. 5.—Comparisons of (a) the Monte Carlo energy distribution with the corresponding Maxwellian distribution of the same mean energy for V = 490 V and pd = 1.4 torr cm, and (b) two Monte Carlo energy distributions for the indicated values of V.

### (a) Mean Energy

Figure 4 shows the variation of the mean energy of the group of electrons as it progresses from cathode to anode. For constant E/p (= V/pd), increasing voltage corresponds to increasing distance provided p is maintained constant, and it can be seen that equilibrium does not appear to be achieved until the applied voltage is  $\sim 400$  V. This value is much greater than can be applied in the actual experimental situation where secondary ionization leads to breakdown at smaller voltages. Consequently one must conclude that in the experimental situations in Sections II and III the mean energy of the swarm of electrons does not in fact settle into equilibrium with the applied electric field.

However, as far as the growth of current is concerned, the significant information must be the distribution of electron energies about the mean value, and this is shown for V = 490 V in Figure 5(a). For comparison, the corresponding Maxwellian distribution for the same mean energy is shown, the peak of the distributions occurring at about the same energy in each case and being larger for the computed distribution than for the Maxwellian. The higher peak is seen to be compensated by a corresponding decrease in the numbers of electrons with energies between about 40 and 140 eV. Since this range of energies corresponds to the peak in the variation of the probability of ionization with energy, this suggests that the re-distribution is a consequence of the efficiency of the ionization process for electrons in this energy range.

In Figure 5(b) a direct comparison is made of the two computed distributions corresponding to V = 165 and 490 V. Allowing for the limitations on accuracy of the low voltage computation in this preliminary study, it can be seen that, despite a large difference in mean energy, the general forms of the distribution function to which computed values of  $\alpha$  will be sensitive are not very different.

### (b) Ionization Coefficient

In order to check the significance of these effects on the ionization coefficient, the values of the current amplification  $I/I_0$  obtained from the Monte Carlo calculations were used to deduce the spatial variation, if any, of  $\alpha(x)$ . For this purpose it was assumed that

$$I(d)/I_0 = \exp\left(\int_0^d \alpha(x) \, \mathrm{d}x\right),\tag{4}$$

from which

$$\int_0^d \alpha(x) \, \mathrm{d}x = \ln\{I(d)/I_0\} \,. \tag{5}$$

Since

$$\ln\{I(d_2)/I_0\} - \ln\{I(d_1)/I_0\} = \int_0^{d_2} \alpha(x) \, \mathrm{d}x - \int_0^{d_1} \alpha(x) \, \mathrm{d}x \,, \tag{6}$$

it is possible in principle to obtain values for  $\alpha(x)$  for small intervals  $d_1$  to  $d_2$  throughout the whole range of distance up to the gap separation d. The results of such an analysis in Figure 6 show that  $\alpha(x)$  does not attain any measure of constancy until the product pd is greater than 0.2 torr cm or  $V \gtrsim 70$  V. This agrees well with the value estimated in the earlier study of Haydon and Robertson (1961), who found they could obtain consistent values of  $\alpha/p$  only by excluding from their analysis all measurements of ionization currents made at voltages less than 70 V.

Considering the simplifying assumptions and the preliminary nature of the present investigation, the saturation value of  $\alpha/p \sim 3 \cdot 2$  is satisfactorily in agreement with the value  $\sim 2 \cdot 6$  deduced from a Gosseries analysis of the experimental growth of current. More detailed investigations, at present in progress, and which consider

actual non-isotropic scattering data for all electron energies rather than on a group basis as in Section IV, indicate values of  $\alpha/p$  closer to those actually measured.

One further observation is worthy of comment. The plot of  $\ln I$  against d which was a straight line of slope 3.2, also intercepted the d axis at a value of d = 0.08 cm. This can be interpreted in terms of the non-equilibrium distance  $d_0$  of equation (1) as

$$\int_0^d \alpha(x) \, \mathrm{d}x \equiv \alpha_{\rm c}(d - d_0) \,, \tag{7}$$

where  $d_0$  is now 0.08 cm and  $\alpha_c = 3.2$ . Over this region up to  $d_0$ , no ionization is assumed to occur. Any variations of  $d_0$  from 0.08 cm lead to values of  $\alpha_c(d-d_0)$  that differ significantly from the values obtained from the Monte Carlo program.



Fig. 6.—Variation with the potential V of incremental values of the ionization coefficient  $\alpha/p$  appropriate to a particular position (or V) in the gap.

This treatment, represented graphically in Figure 7 is a good illustration of the model for the  $d_0$  concept discussed briefly in Section II. As can be seen from Figure 7(b), which shows the small distance region on an enlarged scale, no ionization occurs until d > 0.05 cm. Equilibrium is achieved only when  $d > d'_0 \sim 0.15$  cm and the equivalent situation is represented by  $d_0 \sim 0.08$  cm. Analysis of ionization data obtained in the range  $d < d'_0$  can lead to incorrect values for  $\alpha/p$ , as seen in the next section.

### VI. Gosseries Analysis of Monte Carlo Data

It remains now to analyse the Monte Carlo (I, d) calculations using the same analytical procedure followed with the measured ionization currents, and to compare the general shapes of the curves obtained in the two cases. Figure 8 represents a Gosseries plot of the data shown in Figure 7(a) and includes values of currents calculated for the whole range of V up to 490 V (i.e.  $V \gg V_s \sim 250$  V observed experimentally). The form of the Gosseries equation for this special case, where only primary ionization is considered, is

$$Y_{d} = Y_{d+\Delta d} \exp\left(\int_{d}^{d+\Delta d} \alpha(x) \, \mathrm{d}x\right). \tag{8}$$

Whereas in previous discussions of experimental results, departure from linearity

has been difficult to interpret because this could be due to variations in  $I_0$ ,  $\omega/\alpha$ , or  $\alpha$ , it is now possible with the Monte Carlo data to attribute any curvature directly to variations of  $\alpha$  with electrode separation x. This means that the non-equilibrium effect revealed at small separations in Figure 8 is due simply to  $\alpha$  increasing with increasing gap separation. Of special interest is the fact that linearity is achieved only when currents calculated for voltages  $\gtrsim 70$  V are considered in the analysis. With this restriction, which corresponds almost exactly to that imposed in the analysis of earlier work (Haydon and Robertson 1961), the value for the constant equilibrium value of  $\alpha$  was  $3 \cdot 2$ .





Fig. 7.—Semilogarithmic plot (a) of Monte Carlo currents  $I/I_0$  as a function of pd; the inset (b) shows an enlargement of the small gap situation illustrating the non-equilibrium model.

Fig. 8.—Gosseries plot of the data shown in Figure 7(a). The  $\Delta pd$  values (torr cm) are indicated.

#### VII. CONCLUSIONS

This preliminary Monte Carlo investigation of ionization growth for non-equilibrium conditions has shown that, for conditions appropriate to E/p = 350 V cm<sup>-1</sup> torr<sup>-1</sup> in hydrogen, the mean energy of the electron swarm does in fact vary across the ionization gap. However, in contrast to the mean energy, the primary ionization coefficient is found to settle down fairly quickly to a quasi-equilibrium value. Although the value obtained in the present calculation is rather higher than that observed experimentally, the comparison must be considered satisfactory in relation to the simplifying assumptions which have so far been made.

The observed curvature in the Gosseries plots of experimental data appear also in similar analyses of the Monte Carlo data, showing that the effects can be explained entirely in terms of the spatial variation of the ionization coefficient. This variation

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also verifies the nature of the equilibrium model underlying the use of the well-known Townsend ionization growth equation for determining ionization coefficients. It seems clear that at least part of the explanation for the many discrepancies in ionization data arises from a lack of appreciation of this equilibrium model.

Fortunately, the situation at  $E/p = 350 \text{ V cm}^{-1} \text{ torr}^{-1}$  was sufficiently nonequilibrium to show significant effects on a Monte Carlo analysis. The fact that the predicted non-equilibrium phenomena agree well with those observed should encourage further work to extend the calculations to the extremely non-equilibrium situations at very high values of  $E/p \gtrsim 800 \text{ V cm}^{-1} \text{ torr}^{-1}$ .

While this preliminary investigation has resolved many of the uncertainties surrounding the analysis of ionization currents, further studies which include consideration of the secondary processes are needed.

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