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Monte Carlo Simulation to Study Streamer Theory in Electronegative Gases

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ABSTRACT - Electron swarm motion across a uniform electric field is calculated and analyzed by a Monte Carlo simulation (MCS) method in the presence of elastic excitation, ionization and attachment collisions cross-section with the electronegative gas. The calculation is carried out for a wide range of E/N values from 71 to 1000Td. It is shown that in the case of a steady –state experiment. The motion has been analyzed to give swarm parameters for (drift velocity, number density, mean energy, and effective ionization coefficient). The first aim of the present paper is to calculate the swarm characteristic at 71 Td by MCS and to discuss the difficulty of calculation al low E/N. The second aim is to calculate the swarm parameter for experimental conditions, i.e., the steady state Townsend (SST). The present results are in excellent an agreement with those deduced by the Boltzmann equation analysis for steady- state and pulse Townsend experiments.

Keywords: Monte Carlo method, Electrical discharge, steady state Townsend, Electronegative gases.

1. INTRODUCTION

Detailed investigation into the properties of electron avalanches in gases is necessary since various important modern applications have been developed in the fields of gaseous electronics, electrical engineering and environmental engineering. These applications require a thorough understanding of fundamental principles.

Streamer theory is used to explain breakdown in the absence of significant secondary processes. There are two requirements for the initiation and propagation of a streamer:

1- photons from the avalanche head produce free electrons in the gas by photo ionization (or perhaps by photo detachment from negative ions) .
2- the space charge produced in the avalanche causes sufficient distortion of the electric field that those free electrons move towards the avalanche head , and in so doing generate further avalanches in a process that rapidly becomes cumulative .

The electrons in the avalanche can be assumed to have a roughly spherical distribution, the radius of the sphere being determined by diffusion

The field will be enhanced in front of the head of avalanche, and some of the field lines from the anode will terminate in this head. Behind the head of the avalanche, the field between the electrons and the ions is in the opposite direction to the applied field, and the resultant field strength here is less than the applied electric field strength E. Still further back, the field between the cathode and the positive ions is enhanced again.

In the present paper, the properties of electron avalanches in electronegative gases are studied using a Monte Carlo simulation technique at ratios of the electric field intensity to the gas number density E/N from 71 to 1000 Td(1 Td =1x 10^{-17} Vcm^2= 0.354 V cm^{-1} $Torr^{-1}$ at 0 ^oC).

The values of electron swarm parameters are obtained for steady –state Townsend (SST) experiments, by applying sampling techniques appropriate. In an SST experiment, a constant number of electrons is emitted at the cathode, which generates a steady stream of electrons in the uniform electric field between parallel plates.

Many studies on the electron swarm development in a gases by the Boltzmann equation (BE) method have been reported,[1,2,3,4], while there many investigations by Monte Carlo Simulation (MCS) have been published ; these include works by[5,6,7]. In electronegative gases are a strongly electron attaching gas at low E/N and a strongly ionizing gas at high E/N, so electrons injected into drift space disappear very fast as a result of large attachment at low E/N and the electron number increases rapidly as a result of large ionization at high E/N. Thus, considerable computing time is necessary in order to obtain an accurate results by a MCS at both low and high E/N.

2- MONTE CARLO TECHNIQUE

Monte Carlo technique have been used to simulate electron swarm motion across

uniform electric fields in the presence of both elastic and inelastic collisions. A set of cross – sections including 37 collision processes (elastic, excitation process (electronic and vibration excitation, ionization, attachment)

To simulate a steady –state Townsend (SST) experiment, initial electrons should be generated continuously at the cathode for a time long enough to set up a steady stream of electrons. However, since this is an extremely time-consuming computation, the SST parameters are determined here by sampling appropriate quantities of each type of electron traveling in an isolated avalanche which is started by initial electrons at the cathode. The principles are described below. To obtain the swarm parameters for a SST experiment, the following formula is used:

$$\bar{\xi}(x) = \frac{1}{N_x} \sum_{j=1}^{N_x} \xi_j \qquad (1)$$

Where ξ_j is the value of the quantity to be sampled when the jth electron is contained in a small region between x and x+Δx and N_x is the total number of electrons that appear there. These electrons moving both forward (x direction) and backward (-x direction) are sampled and $\bar{\xi}(x)$ averaged gives the local value at x[8], where x is the position in the inverse field direction.

In order to define clearly the different swarm parameters which are calculated in the present work let us consider a swarm of electrons released at time t=0 initial of electrons, the number of which is **g** are released to the drift space from the origin and we pursue each electron from t=0 to simulation time t_f . The values of **g** and t_f depend on E/N.

The gas number density N is assumed equal to 3.54×10^{16} cm^{-3} (1Torr at 0 ^oC) . The collisions between electron and gas molecules only are considered; both Coulomb interaction between charged particles and the effect of electron detachment from negative ions are neglected.

3- RESULTS AND DISCUSSION

The electron density variation between parallel plats**.** The consideration in equation (1) shows that the local electron density may be sampled as:

$$n(x) = g \sum_j \Delta t_j / \Delta x \qquad (2)$$

Where, g is the number of initial electrons per second released at the cathode in a steady state and Δt_j , the mesh width in time.

The variation of electron density n(x) is shown in figure (1). n(x) is seen to increase exponentially with the distance from the cathode.

Figure (2), shows the variation of the electron swarm parameters for SST as function of the distance x from the cathode for many values of E/N. The initial distribution is an isotropic Maxwellian with a mean energy of 9.8 eV. The points in the figure indicate the average values at the respective positions. The present simulation is performed without considering the effect of the electrode. And the variation of the electron energy distribution F(ε, x) between parallel plates may be sampled by putting ξ_j in equation (1) equal to unity if the jth electron has an energy between ε and ε+ Δ ε ; otherwise ξ_j=0.

To determine the localized electron mean energy $\bar{\varepsilon}$ accurately from equation (1) , Δx should be small and **g** should be large . In the present work Δx was chosen to be 0.005 cm and **g** a few tens of thousands to reduce the statistical fluctuation in ε (x) to less than about 0.1 eV. Retaining such a large **g** for positions near the cathode required to start a large number of avalanches from the cathode and to terminate these avalanches in the midway to the anode for economizing computer time without giving any influence to the results. This was done by tracing electrons which belong to an avalanche until the confirmation was made that no one of them could reach by back scattering the terminating position x.

Fig.(3),represent the effective ionization coefficient $\bar{\alpha} = \alpha - \eta$ is deduced from the slope of (-ln (n(x)/g)) against x , from this figure since α is the ionization , and η the electron attachment coefficients . the calculation becomes much more difficult at lower E/N values because η is larger (because of attachment electron at low energy and consist negative ion).

Figure (4) the electron drift velocity V_d is shown as a function of a distance of cathode the electron velocity is increases with increases the values of E/N. The electron undergo changes in distribution function due mainly to inelastic collisions which are the vibrational excitation, electronic excitation and ionization. Figure (5) shows the variation of the electron swarm parameters for SST with respect to (x) at values of E/N =141 and 566 Td. The initial distribution is an isotropic Maxwellian with a mean energy of 9.5 eV.

The values of drift velocity V_d for various E/N are shown in table 1 with those calculated from Boltzmann equation for comparison . The results deduced from MC & BE are in good agreement for all the E/N.

Table(1):- Values of electron swarm parameters in Electronegative gases for various E/N calculated from MC & BE (A gas number density of 3.45×10^{16} cm^{-3} (1 Torr at 0 ^{o}C is assumed).

SST				
E/N(Td)	***Method***	$\bar{\alpha}$ ***(cm^{-1})***	***$V_d x10^6$ ($cm.s^{-1}$)***	$\bar{\varepsilon}$ ***(eV)***
141	***MC***	***-3***	***9.5***	***5.3***
	B E	***-2.6***	***10***	***5.6***
566	***MC***	***2.25***	***30***	***9.3***
	B E	***2.1***	***26***	***9***

- MC, Monte Carlo Method (in the present work); BE , two term expansion Boltzmann equation [2].

When the E/N values are less than 141 Td the Boltzmann equation method become unstable. and so we employ a Monte Carlo Simulation method at such low E/N . However, considerable computing time is necessary to obtains results by a Monte Carlo simulation, because electrons injected into drift space disappear very quickly due to the large electrons attaching probability at low electron energy. As a consequence the present simulation is performed only at 71 Td.

The calculation have been achieved by: (computer program for solution of Monte Carlo Method) has been written in MATLAB PROGRAM VERSION 6.5).

4- CONCLUSION

The Monte Carlo simulation of electron swarm motion has confirmed the model arising from the solution to Boltzmann's equation. A **MCS** has been performed for electron swarms in electronegative gases for E/N from 71 to 1000Td. A set of electron collision cross sections determined in a previous study of [3], was used. The principle of observation of the electron swarm, i.e., the steady state Townsend (**SST**) was considered.

The electron swarm parameters and electron energy distribution in the present work are in excellent agreement with those deduced in the previous study.

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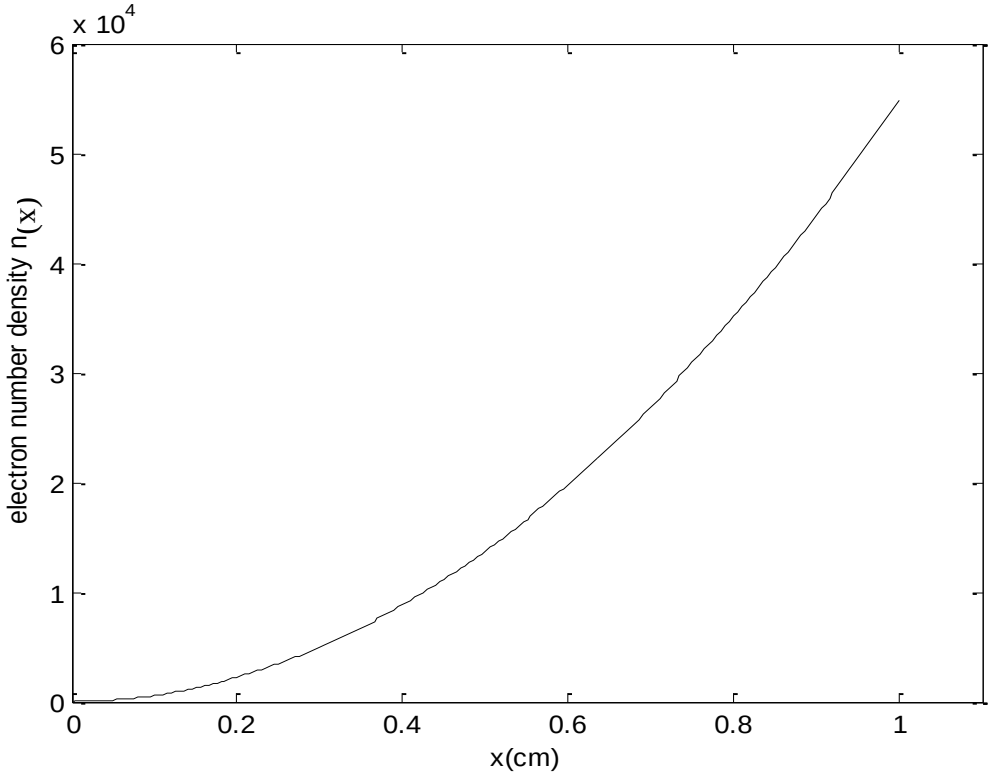

Fig. (1):- The variation of the electron number density n(x) as a function of the distance x from the cathode.

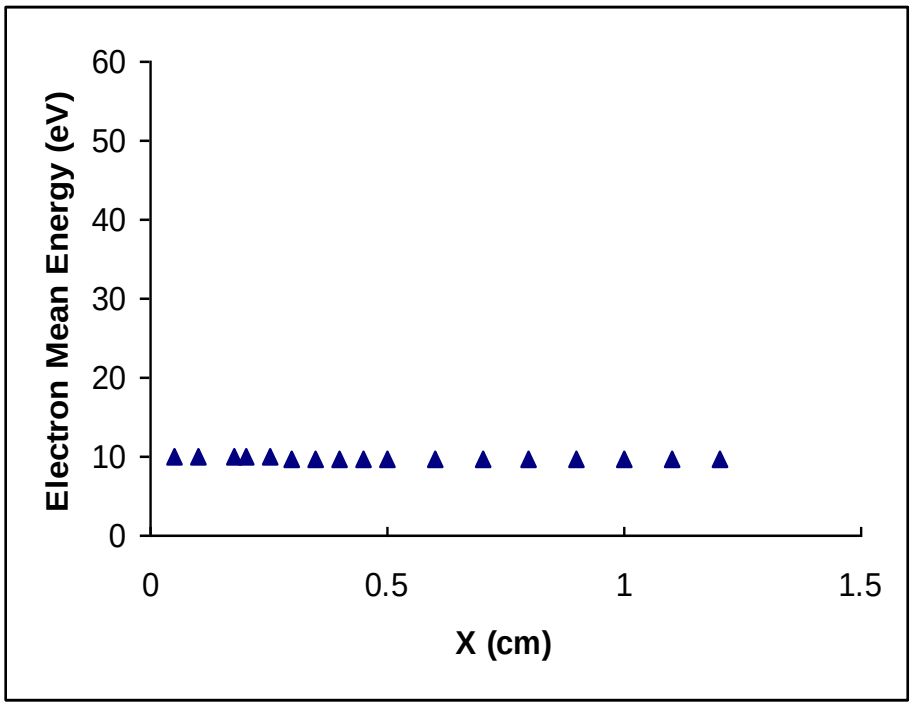

Fig.(2):- The variation of the SST parameters (electron mean energy $\bar{\varepsilon}$) as a function of the distance x from the cathode.

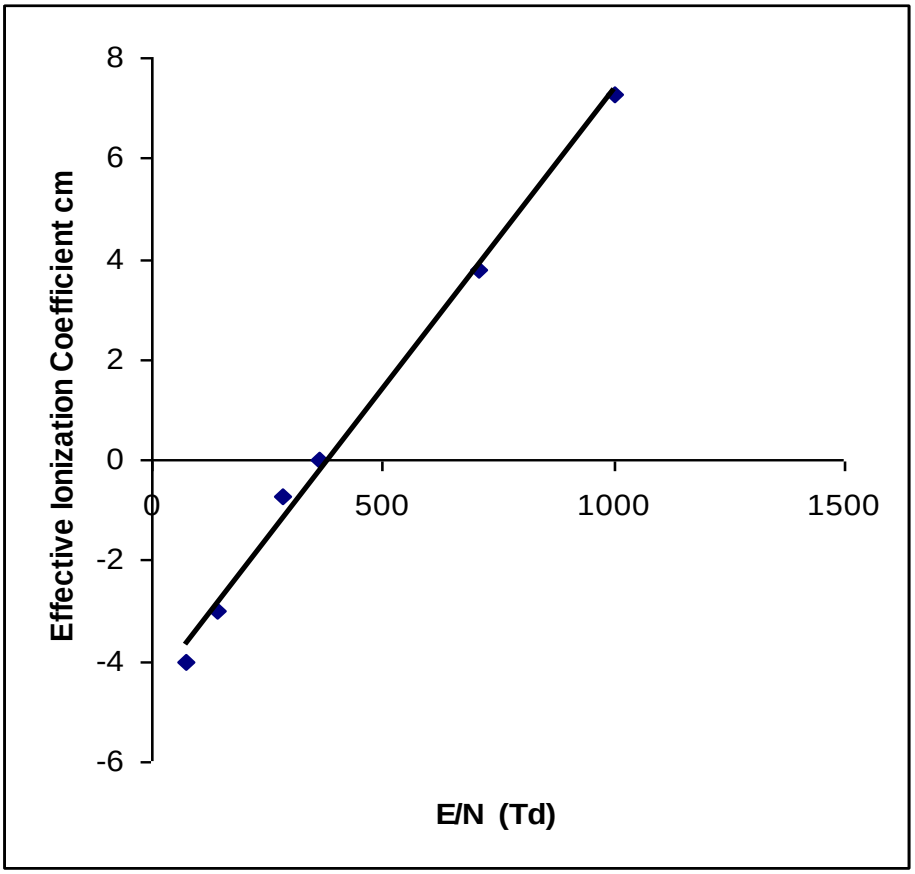

Fig.(3):- effective ionization coefficient as a function of E/N , ♦ present work (Monte Carlo simulation), _____ two term Boltzmann Equation[3] .

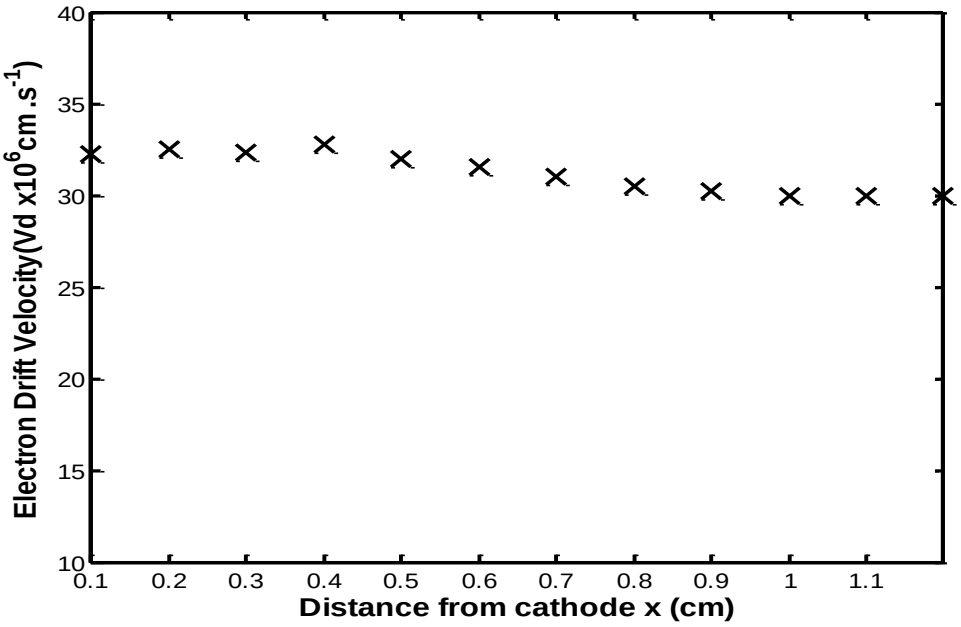

Fig. (4):- The variation of the SST parameters (electron drift velocity V_d) as a function of the distance x from the cathode.

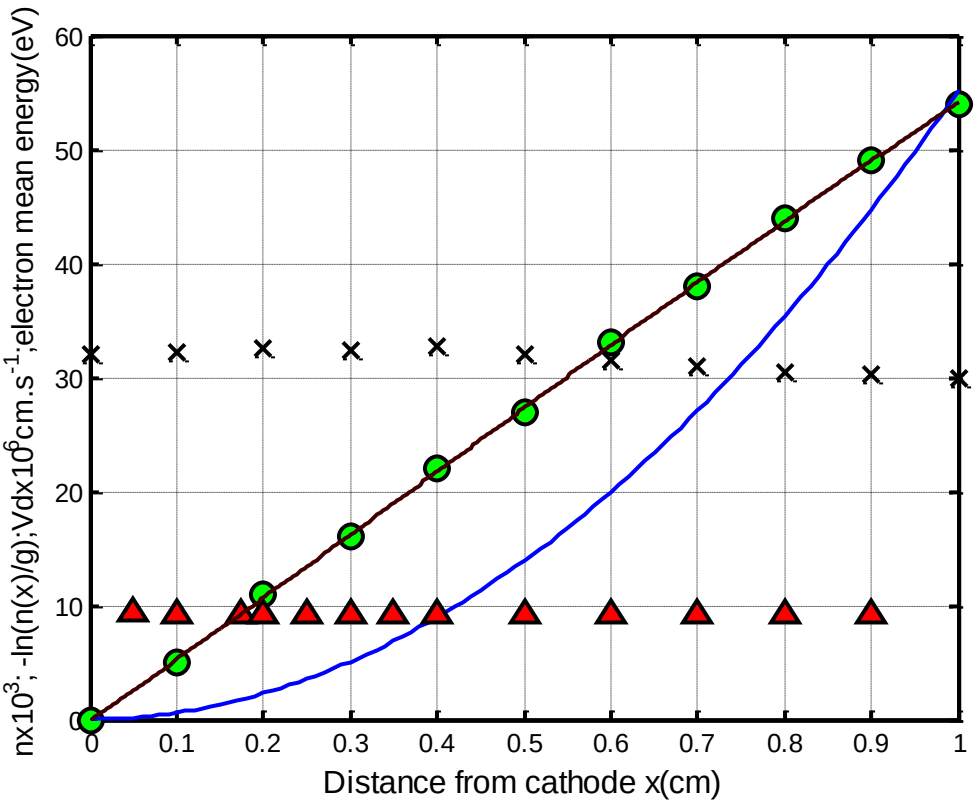

Fig.(5):- The variation of the SST parameters as a function of the distance from the cathode : (solid line)electron number density n(x); (O) (-ln(n(x)/g)); **(x)** V_d**; (▲)** $\bar{\varepsilon}$ **.**

استخدام طريقة Monte Carlo Simulation لدراسة نظرية سيل حشد الالكترونات في الغازات الكهروسالبية

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الخلاصة

لدراسة تحليل معلمات حشد الإلكترون في الغازات الكهروسالبية بوجود مجال كهربائي منتظم , نستخدم طريقة (Monte Carlo simulation) , بوجود نوعين من التصادمات والتي هي : أولا التصادمات المرنة وثانيا التصادمات الغير مرنة والمتمثلة بـ (المقطع العرضي للتصادم التأين, الارتباط والتهيج...الخ) , الحسابات أنجزت المدى قيم E/N من ٧١ إلى ١٠٠٠ تاونزيند , تحت شرط الحالة التجريبية . Steady –State Townsend

تحليل حركة حشد الإلكترون أعطى بعض المعلمات والتي هي (سرعة الانجراف, الكثافة العددية, متوسط الطاقة الحركية, و معامل التأين المؤثر).

الهدف الأول من البحث هو توصيف معلمات الحشد في ٧١ تاونزيند بطريقة Monte Carlo simulation وهي قيمة قليلة يصعب حسابها بطريقة أخرى , والهدف الثاني هو حساب معلمات حشد الإلكترون تحت شرط SST, وبينت النتائج أن هناك تطابق مع النتائج التي تم دراستها بطريقة معادلة بولتزمان.