Numerical Study for Pure Nitrogen Gas Discharge

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Abstract :

A theoretical approach for calculating the Electron Energy Distribution Function (EEDF) and electron transport parameters (ionization and diffusion coefficients, drift velocity, mobility, characteristic energy and electron mean energy) has been established in a weakly ionized pure nitrogen (N_2) which investigated for the steady-state conditions. With in this approach, the effect of the reduced electric field strength (E/N) on these parameter have been studied and calculated numerically for a wide range of (E/N) from ((0.1-200)Td) (1Td = 10^{-17} V.cm^2 =0.354 V.cm^{-1}.torr^{-1} at 0 ^{o}C) by using the two-term Boltzmann Transport Equation (BTE) approximation method. The excellent agreement of the present result with the other published data according to the proposed cross section. These analyses are carried out using a constructed computer code and a Matlab (version: 7.6.0.324 (R2008a)) scientific software.

Keywords: Glow discharge, pure nitrogen, EEDF.

Introduction :

A number of investigators has been carried out a theoretical calculations on the electron swarm parameters and electron energy distribution function (EEDF) in a weakly ionized gases by using Boltzmann transport equation (BTE) method. For example: H. Itoh, et. al., 1990, computed the electron swarm parameters for a ramp model gas and argon for selected values of (E/N) by using three-term approximation. Braglia, et. al., 1990, showed that there is no change in all the transport parameters of mercury when passing from two-term to four-term expansion. Al-Amin, et. al., 1985, measured the characteristic energy for (CO, N_2, H_2) with the covering a wide range of (E/N) from (2.8 x 10^{-16} to 5.65 x 10^{14} V.cm^2). Li and Chen,1993, showed that the three-term expansion of distribution function will added a very small part to the first term of (BE) that was derived by Frost and Phelps,1962, which represent the inelastic cross-section and can be neglected.

The role of electron transport parameters are an important because it provides a link between electron-gas collision cross-section, gas breakdown discharge phenomena and the modeling of the glow discharge which is in such devices: gas lasers, lamps, electron beam sources and plasma panels. [Raizer, 1991] [Bittencourt, 1986].

In electron transport parameters calculation, the reduced electric field strength (E/N) is a critical parameter that imposes variations on the characteristics of the electron swarms in (N_2), these parameters can be calculated directly from a set of collision cross-section by using either (BE) or Monte Carlo completely simulation method[Tagashira, et. al.,1976], so the product of such calculation is the (EEDF), which is the key and very important in helping to evaluate the electron mean energy, drift velocity, mobility, ionization and diffusion coefficient and characteristic energy.

This paper presents a theoretical investigation of the effect of (E/N) on the electron transport parameter in pure (N_2) over a wide range of reasonably practical conditions.

Theoretical consideration:

The behavior of electron interactions with gas molecules are governed by the distribution in space, energy and time of the electrons in pure gases or in a mixture of gases. The main objective of (BTE) is to predict this distribution which is expressed as f($\vec{r},\vec{v},t$).The general form of (BTE) may be written as [Huxley and Crompton, 1974][Gnudi, et. Al., 1993] :

$$\frac{\partial f(\vec{r},\vec{v},t)}{\partial t}+\vec{V}.\nabla_r f(\vec{r},\vec{v},t)+\frac{eE}{m}\nabla_v f(\vec{r},\vec{v},t)=\left(\frac{\partial f}{\partial t}\right)_{coll.} \quad ....(1)$$

Where $f(\vec{r},\vec{v},t)$ is the electron velocity distribution function (EVDF) at spatial location ($\vec{r}$) at time (t). $\frac{e}{m}$ is the ratio of electronic charge to the electron mass and E electric field, $\vec{V}$ velocity vector. The first-term on the left side of Equ.(1) gives the local variation of the distribution function with time, the second-term describes the variation in the distribution function resulting from electron streaming in and out of a given volume elements. This term is closely related to the description of diffusion, the third-term is the variation of the distribution function resulting from applied electric field (E) acting on the electron. The single-term on right-hand side accounts for the net transfer from the differential volume by the mechanism of binary collisions between electrons and molecules, ions, and other electrons, we made the following simplification in order to streamline the computation effort. In the case of a spatially uniform gas [Eiichi, et., al., 2007 [Filbert, 2003] :

$f(\vec{r},\vec{v},t)\rightarrow f(\vec{v},t)$; i . e There are no spatial gradient of the $\vec{E},n_e$ $\rightarrow \nabla_r f=0$

So that the equation (1) become :

$$\frac{\partial f}{\partial t}-\frac{eE}{m}\nabla_v f=\left(\frac{\partial f}{\partial t}\right)_{coll.} \quad ....(2)$$

The multi-term expansion of the Electron Velocity Distribution Function (EVDF) (f) in spherical harmonics takes the form

$$f(\vec{r},\vec{v},t)=\sum_{n=0}^{\infty} f_n(\vec{r},\vec{v},t)P_n(\cos\theta)...(3)$$

$$f(\vec{v})= f_0(\vec{v})+\sum_{n=1}^{\infty} f_n(\vec{v})P_n(\cos\theta)....(4)$$

$$f(\vec{v})= f_0(\vec{v})+ f_1(\vec{v})P_1(\cos\theta)+ f_2(\vec{v})P_2(\cos\theta)+ f_3(\vec{v})P_3(\cos\theta...(5)$$

The deflections of electrons during the collisions process are large because of the large difference between the mass of electrons and the gas atoms or molecules. In this case the (EVDF) ($f(\vec{v})$) is almost independent of the direction of v, that is [Holstein, 1946].

$$f(\vec{v}) \approx f_0(\vec{v})+\frac{\vec{v}}{v}.f_1(\vec{v}).....(6)$$

Where f_0, f_1 are functions of v (the magnitude of $\vec{v}$ only) and $f_1 << f_0$, where f_0 is isotropic and f_1 is a small anisotropic part. The expansion of Equ.(6) is to be substituted in Equ.(2), then Equ.(2) may be resolved into the two coupled equations :

$$\frac{\partial f_1}{\partial t}-\frac{eE}{m}\frac{\partial f_o}{\partial v}=\left(\frac{\partial f_1}{\partial t}\right)_{coll.} .....(7)$$

$$\frac{\partial f_0}{\partial t}-\frac{e}{3m}.\frac{E}{v^2}\frac{\partial}{\partial v}(v^2 f_1)=\left(\frac{\partial f_0}{\partial t}\right)...(8)$$

An electron-heavy particle momentum-transfer collisions play the major role in reducing the asymmetry in the distribution function. Therefore, the right hand side of Equ.(7) has a particularly simple form, that is [Holstein, 1946] [Smith and Thompson, 1978] :

$$\left(\frac{\partial f_1}{\partial t}\right)_{coll.}=-\nu_{ej}(v)f_1(v)$$

Where $\nu_{ej}(v)$ is the electron momentum transfer collision frequency for the j[th] species of heavy particles and momentum transfer cross section by the expression.

$$\nu_{e\alpha}=N_\alpha\sigma_{m\alpha}(v)v$$

Then

$$\left(\frac{\partial f_1}{\partial t}\right)_{coll.}=-N\sigma_{m\alpha}(v)vf_1(v) \quad ...(9)$$

Using Equs. (7-9), an equation for the isotropic of f(v) can be obtained. After transformation to the new independent variable :

$$\in=\frac{mv^2}{2e}$$

Where, ($\in$) is the electron energy in (eV) making a change in the independent variable :

so that :

$$\frac{\partial}{\partial v}=\frac{\partial \in}{\partial v}.\frac{\partial}{\partial \in}=\frac{mv}{e}.\frac{\partial}{\partial \in}$$

We get :

$$\frac{\partial f_0}{\partial t}-\frac{2e}{mv}.\frac{\partial}{\partial \in}\left[\frac{\in^2}{3N\sigma m}.\frac{\partial f_0}{\partial \in}+2\frac{m}{m}n\sigma_m \in^2 f_0+2\frac{mk_BT}{Me}N\sigma_m \in^2 \frac{\partial f_0}{\partial \in}\right]$$

$$=\left(\frac{\partial f_0}{\partial t}\right)_{Coll.} \quad ...(10)$$

In Equ. (10)

$f_0(\in)$: Normalized EEDF

$$\int_0^{\in} f_0(\in)d\in=1^{1/2}$$

E : Applied electric field (V.cm^{-1})

N : Total molecular no. density (cm^{-3})□□□$_m$: Momentum transfer cross-section for elastic collisions (cm^2).

K_B : Boltzmann constant

T : Gas temp.

The right hand side of equ.(10) represents the combined effect on the distribution function f($\in$) of superelastic and inelastic electron-neutral collisions[Paniccia,et. Al.,1988] [Perthame,2004] :

$$\left(\frac{\partial f_0}{\partial t}\right)_c=\left(\frac{\partial f_0}{\partial t}\right)_i+\left(\frac{\partial f_0}{\partial t}\right)_s ...(11)$$

Where $\left(\frac{\partial f_0}{\partial t}\right)_i$ is the contribution due to inelastic collisions.

$\left(\frac{\partial f_0}{\partial t}\right)_s$ is the contribution due to superelastic collisions.

The analysis of the effect on f($\in$) of such collisions, which the energy exchange is an appreciable function of the electron energy, is

$$\left(\frac{\partial f_0}{\partial t}\right)_i=\sum_i N_0\left[f_0(\in+\in_i)\sigma_i(\in+\in_i)-f_0(\in)\sigma_i(\in)\in\right]\frac{2e}{mv}...(12)$$

The contribution to $\left(\frac{\partial f_0}{\partial t}\right)_s$ is expressed as

$$\left(\frac{\partial f_0}{\partial t}\right)_s=\sum_j N_j\left[f_o(\in-\in_j)\sigma_j(\in-\in_j)(\in-\in_j)-f_o(\in)\sigma_j(\in)\in\right]\frac{2e}{mv}.....(13)$$

N_j : no. of molecules in the j[th] excited state ; hence

$$N = N_o + \sum_j N_j$$

From Equs. (10-13) we get :

$$\left(\frac{m\in}{2e}\right)^{1/2}\frac{\partial f_o}{\partial t}=\frac{E^2}{3}.\frac{\partial}{\partial\in}\left[\frac{\in}{N\sigma_m}.\frac{\partial f_o}{\partial\in}\right]+\frac{2m}{M}\frac{\partial}{\partial\in}\left(\in^2 N\sigma_m f_o\right)+$$

$$\frac{2mKT}{Me}.\frac{\partial}{\partial\in}\left(\in^2 N\sigma_m f_o\right)+\sum_j\left[(\in+\in_j)f_o(\in+\in_j)N_o\sigma_j(\in+\in_j)-\in f(\in)N_0\sigma_j(\in)\right]+$$

$$\sum_j\left[(\in+\in_j)f_o(\in+\in_j)N_o\sigma_j(\in+\in_j)\in f_0(\in)N_j\sigma_{-j}(\in)\right] \quad ...(14)$$

$\in_j$: Energy loss in (volts) for the j[th] inelastic process in species

□$_j$: is the elastic cross-section(vibration, excitation, electronic excitation, ionization for this process (cm^2))

□$_{-j}$: Cross-section (cm^2) for superelastic collisions

$$\sigma_{-j}=(\in+\in_j)\sigma_j(\in+\in_j)$$

In the case of steady-state dividing by N and integrating once, we get a first order integral differential equation.

$$\frac{1}{3}\left(E/N\right)^2 \frac{\in}{\sigma_m(\in)}\frac{df_0}{d\in}+\frac{2m}{M}\in^2\sigma_m(\in)fo+\frac{2mK_BT}{Me}\in\ \sigma_m\frac{df_o}{d\in}+\sum_j\int_0^{\in j}d\in' \quad \text{Equ.(}$$

$$\left[(\in+\in')\sigma_j(\in+\in')f_o(\in+\in')+(\in-\in')\sigma_{-j}(\in-\in')\frac{N_j}{N}\right]=0 \quad ..(15)$$

15) apply to electron in a gas of one type of molecules for a specific value (E/N) .EEDF is determined by solution of Equ.(15).

Method of solution :

BTE is analytically formulated for isotropic distribution then the application of finite difference method which convert the differential terms to difference terms is given and finally the method for solving the set of equations by matrix method. BE in a two term approximation is indicating in Equ. (15) for pure (N_2) gas. Given the appropriate momentum transfer and a set of cross-sections, we compute the EEDF[Elliot&Green,1976],and electron transport parameters. [Hassani,et.al.,2003]

- Electron mean energy

$$\langle\in\rangle=\frac{2}{3}\int_0^\infty \in^{3/2} f_o(\in)d\in \quad ...(16)$$

- Drift velocity

$$V_d=-\frac{E}{3}\left(\frac{2e}{m}\right)^{1/2}\int_0^\infty\frac{\in}{N\sigma_m}\frac{\partial f_o(\in)}{\partial\in}d\in \quad ....(17)$$

-Ionization coefficient

$$\frac{\alpha}{N}=\frac{1}{Vd}\left(\frac{2e}{m}\right)^{1/2}\int_0^\infty\sigma_i(\in)\in f_o(\in)d\in \quad ...(18)$$

- Diffusion coefficient

$$D=\frac{1}{3}\left(\frac{2e}{m}\right)^{1/2}\int_0^\infty\frac{\in}{N\sigma_m}f_o(\in)d\in \quad ....(19)$$

$$\in_k=\frac{eD}{\mu} \quad ....(20)$$

Where (μ) is the electron mobility for Maxwellian energy distribution function

$$\frac{eD}{\mu}=\left(\frac{2}{3}\right)\in$$

- Characteristic energy

$$\in_k=\frac{eD}{\mu} \quad ....(20)$$

Where (μ) is the electron mobility for Maxwellian energy distribution function

$$\frac{eD}{\mu}=\left(\frac{2}{3}\right)\in$$

In the present calculation we carried out by varying (E/N) from (0.1 Td) to (200 Td) . The gas number density (N) was assumed to be (3.54×10^{16} cm^{-3}) (1 torr at 0^oC).

Results and Discussion :

The (EEDF) has been computed as a function of electron energy ($\in$) by using the two-term Boltzmann Equation approximation method in pure molecular gas (N_2) at different values of (E/N) ((0.01, 0.1, 1.0) Td) as shown in Fig. (1). For the lowest value of (E/N), it appears that the distribution function are sharply peaked at low electron energy and rapidly decrease as it increases, which indicate the domination of the attachment processes and when (E/N) increases, the (EEDF) curves are slightly shifted towards higher energy values with tail broadening and decreasing its maximum value ($f(\in))_{max}$. which attribute, to the decreasing of the attachment processes and increasing the ionization coefficient, as well as having the dominant electron-molecule energy exchange processes. The distribution function at low electric field is namely semi-logarithmically with slope equal $(K_BT)^{-1}$ and this indicates a Maxewellian distribution, while for higher electric field, the distribution become non-Maxewellian because the electrons acquired energy through the applications of an electric field which accelerated and then drift due to the high energy gain, so that the main transport parameters are considered as a function of (E/N) like the drift velocity and the mobility of electrons besides the other transport parameters.

Fig.(2) show a good agreement of theoretical (Equ.(17)) and experimental values of the electron drift velocity [[Morgan & Penetrante,1990], which is a function of (E/N). It appears a linear relation between them at low electron energy and its linearity means the transport obeys ohm' law, where the velocity increases with applied fields. The transition from low field transport to high field transport occurs around (40 Td) approximately and beyond these critical value (at high field) there is no further increasing in drift velocities due to phonon emission by the high energy electrons. Fig.(3) shows the electron mobility as a function of (E/N) (Equ.20) which indicates the decreasing in mobility with increasing (E/N) values during the inelastic collision processes. The behavior of the diffusion coefficient as a function of (E/N) (Equ.19) is shown in Fig.(4). It has the plateau at a range (5-40 Td) and these values low mean energy corresponds to high values of (σ_m) in pure (N_2) and beyond this range the diffusion coefficient increases with increasing (E/N) due to the ear behavior of ionization coefficient ($\frac{\alpha}{N}$) (Eq. (18)) a shown in Fig. (5) for the range ((80-200)Td),which means that the electrons acquired enough energy from the applied electric field to reach the ionization level of pure (N_2)and increases the numbers of energetic electrons. A good agreement has been obtained to the experimental data of Haydon [Haydon & Williams,1976].The variation of mean electron energy $\langle\in\rangle$ (Equ.(16)) with (E/N) is shown in Fig. (6), which in general increases from (0.13eV) at (E/N =0.1 Td) to (4.61 eV) at (E/N = 200 Td).

The extension of the horizontal part in Fig.(6) is intersecting the mean energy axis at appropriate value (0.8 eV). As the field increases, the electron gains more energy from field, and then the mean energy is increasing. Generally the non-linear effects are related to the cases of non-equilibrium distribution.

The characteristic energy Equ. (21) as shown in Fig.(7) is also increases with increasing (E/N) because of elastic collision process(E/N >1 Td) and then starts to be approximately constant during the inelastic collision-process up to (E/N=20 Td),as (E/N) is increasing beyond (E/N=1 Td), ($\in_k$) initially remains bound to value of (2.4 eV), by elastic losses in the large barrier of (σ_m). A good agreement has been obtained with published data of Huxley [Huxley & Crompton,1974] in the elastic region and be larger than Morgan experimental data[Morgan & Penetrante,1990].

acquired high energy from the high electric field which raised its diffusion. The non-linear behavior of ionization coefficient ($\frac{\alpha}{N}$) (Eq. (18)) a shown in Fig. (5) for the range ((80-200)Td),which means that the electrons acquired enough energy from the applied electric field to reach the ionization level of pure (N_2) and increases the numbers of energetic electrons. A good agreement has been obtained to the experimental data of Haydon [Haydon & Williams, 1976]. The variation of mean electron energy $\langle \in \rangle$ (Equ.(16)) with (E/N) is shown in Fig. (6), which in general increases from (0.13 eV) at (E/N =0.1 Td) to (4.61 eV) at (E/N = 200 Td).

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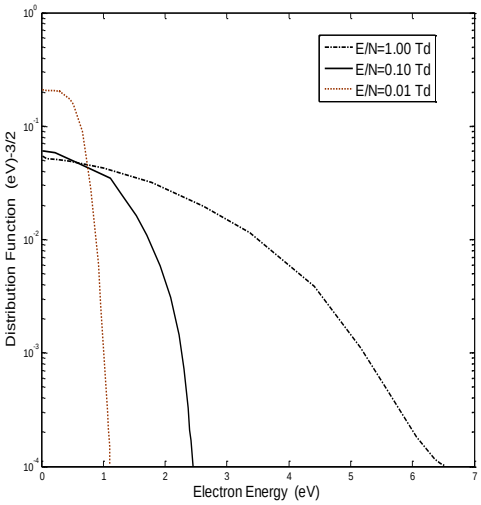

Fig.(1):The electron energy distribution functions as a function of electron energy in pure (N_2) for several values of (E/N).

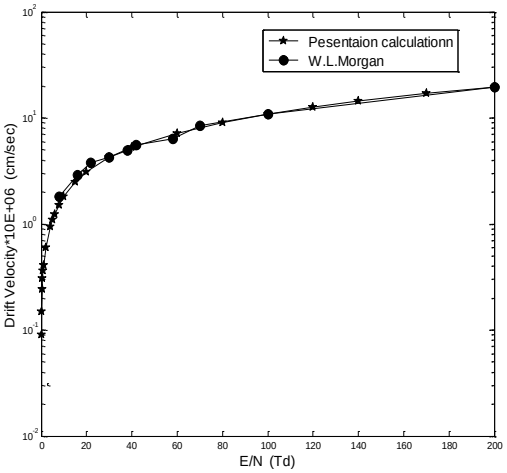

Fig.(2):The drift velocity of electrons as a function of (E/N).

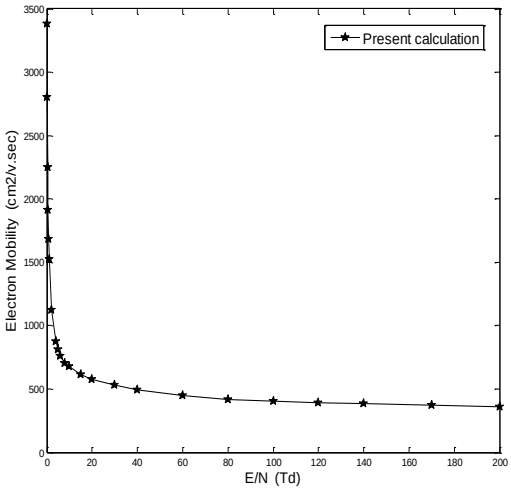

Fig.(3):The mobility of electron as a function of (E/N).

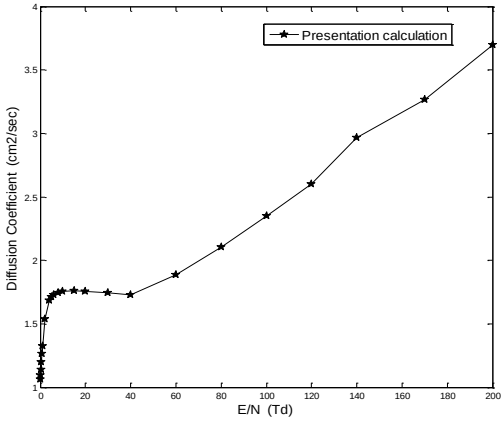

Fig.(4): The diffusion coefficient of electrons as a function of (E/N).

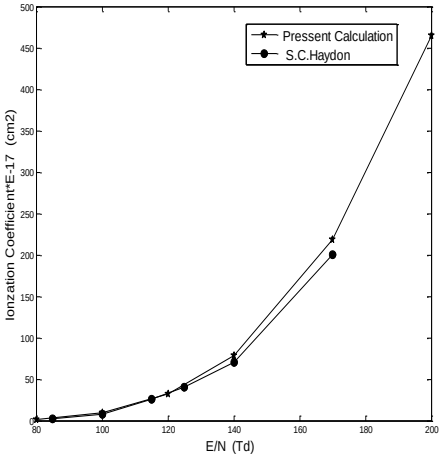

Fig.(5): The ionization coefficient of electrons as a function of (E/N).

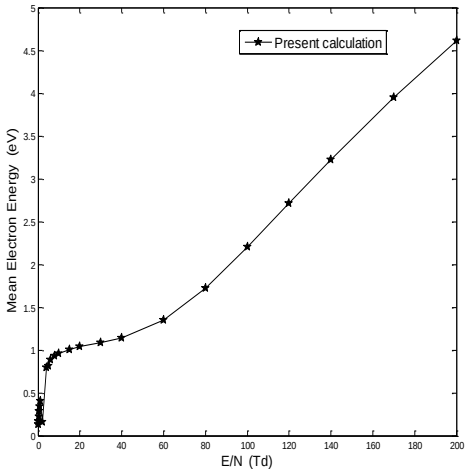

Fig.(6): The mean electron energy of electrons as a function of (E/N).

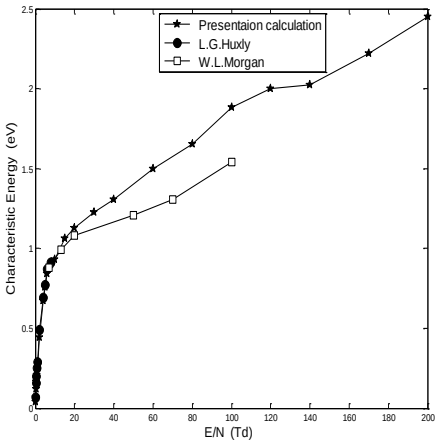

Fig.(7): The characteristic energy of electrons as a function of (E/N).

Conclusion :

We show that the numerical solution of the (BTE) in a two-term spherical harmonics approximation which using the set of cross-section is simple, efficient and is valid to calculate the steady-state electron transport parameters in a weakly ionized gas (N_2) in a hydrodynamic equilibrium. Generally, the accuracy of calculation also depend on the accuracy of the electron-molecules cross-section sets. Calculations of the (EEDF) for discharge process of (N_2) have shown that is highly non-Maxewellian except at very small values of electron energy and the occurrence of the ionization for (N_2) atoms, which means that the electrons acquire the required energy to ionized the N_2-atoms at less (E/N) values.

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دراسة التحليل العددي للتفريغ الغازي للنيتروجين النقي

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(تاريخ الاستلام: ٢٨ / ١٢ / ٢٠٠٩ ---- **تاريخ القبول:** ٢٧ / ٤ / ٢٠١٠ **)**

الملخص:

تم نظريا حساب دالة التوزيع الطاقي للالكترونات (EEDF) ومعلمات الانتقال الالكتروني (معاملات التأين والانتشار الالكتروني،سرعة الانجراف،معدل طاقة الإلكترون ،حركية الإلكترون) لغاز النتروجين النقي ضعيف التأين ،كما تم التحليل العددي لتأثير قوة المجال الكهربائي (E/N) على تلك المعلمات ضمن مدى تأثير هذه القوة ((0.1-200)Td) ($1Td = 10^{-17}$ $V.cm^2$=0.354 $V.cm^{-1}.torr^{-1}$ at 0 ^oC)وبالاستناد إلى طريقة ذي الحدين التقريبية لحل معادلة بولتزمان الانتقالية (تحت شرط الاستقرار) مستفيدين من إمكانيات البرنامج العلمي Matlab (version R2008a) في برمجة العمليات الحسابية ورسم المنحنيات وقد أظهرت النتائج توافقا جيدا مع النتائج النظرية والعملية المنشورة لبعض الباحثين.