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NUMERICAL CALCULATIONS OF THE ELECTRON ENERGY DISTRIBUTION FUNCTION IN (50% SF_6 - 50 % Xe) MIXTURE WITH CORRESPONDING TRANSPORT PARAMETERS

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Abstract

We used EEDF software package program to solve Boltzmann equation to calculate the electron energy distribution function in (50% SF6 – 50% Xe) mixture. The calculations are achieved under a steady state electric field using the classical two - term approximation. The electron energy distribution function (EEDF) and the corresponding transport coefficients (mean electron energy, characteristic energy, mobility of electron, diffusion coefficient, and drift velocity) for constant and various electron concentrations are calculated and graphically represented. It is found that variations of electron concentration have a significant effect on transport coefficients of the mixture. The work is in a well agreement with previously experimental and computational researches.

Keywords: EEDF Program; EEDF; Boltzmann Equation; SF_6-Xe Mixture; Transport Coefficients.

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1. Introduction

EEDF has a substantial role in plasma modeling due to it need for computation the reaction rates for electron collision reactions [1-2]. There are various possibilities that describing the EEDF, such as Maxwellian, Druyvesteyn, a generalized form between the Maxwell and the Druyvesteyn function, and the solution of the Boltzmann equation [3-4]. The distribution functions assume that elastic collisions are dominated; therefore, the effect of inelastic collisions (ionization or excitation) on the distribution function is insignificant [5].

In thermodynamic equilibrium the EEDF has a Maxwellian shape if the ionization degree is high because electron – electron collisions drive the distribution towards a Maxwellian [6]. However, in most of the plasmas the deviations from the Maxwellian shape take place. At higher electron energies the inelastic collisions of electrons with heavy particles play a significant role in the dropping of EEDF. On the other hand, for a lower ionization degree the Druyvesteyn distribution

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function almost often leads to more accurate results. The Maxwellian EEDF is based on constant collision frequency; while the Druyvesteyn EEDF is based on a constant cross section (the electron energy is independent) [7].

The electron transport properties can be derived from EEDF, thus the choice of EEDF would affect the results of plasma model. There are several computational resources and numerical techniques used to find the transport properties [8]. One of them is presented in the EEDF software package [9]. This program gives results of the kinetic and transport coefficients of plasma in the mixture of gases by numerically solving Boltzmann equation of EEDF in low – ionized plasma in an electric field.

It is known that some inert gases such as helium, neon, argon, krypton, xenon and mixtures with some gases, such as chlorine and SF_6, are important in practical applications as in the electrical discharge [10]. Therefore, there is a huge need to have accurate data about the electrical discharge. In this paper we present calculated data for a mixture of (50% SF6 – 50% Xe) under a steady state electric field. The EEDF program is adapted for such calculations of EEDF and electron transport coefficients.

Method of numerical solution in the code

The EEDF can be computed by solving the Boltzmann equation. The latter describes the evolution of the distribution function, in a six – dimensional phase space. The Boltzmann equation under consideration is given by [11]:

$$u^{1/2} f_0(u)(dn_e/dt) = I_{\mathrm{E}}(u) + I_{\mathrm{el}}(u) + I_{\mathrm{in}}(u) + I_{\mathrm{ee}}(u) \quad (1)$$

where u is electron energy, $f_0(u)$ is the isotropic part of the distribution function, the term $I_{\mathrm{E}}(u)$ describes heating of the electrons in the electric field. Terms $I_{\mathrm{el}}(u)$, $I_{\mathrm{in}}(u)$ and $I_{\mathrm{ee}}(u)$ describe elastic, inelastic and electron – electron collisions and dn_e/dt is a term expression for the conservation of the electron density given by [11]

$$dn_e/dt = n_e(\bar{\nu}_{\mathrm{i}} - \nu_{\mathrm{att}} - \nu_{\mathrm{rec}}) \quad (2)$$

where ν_{i}, ν_{att}, ν_{rec} are the frequencies of ionization, attachment and recombination, which can be expressed in terms of appropriate integrals of $f_0(u)$. The EEDF code solves Boltzmann equation for the isotropic part of the electron velocity distribution function in homogeneous plasma numerically using an iterative method. With the condition (2) the code solves Boltzmann equation. Then to calculate $(dn_e/dt)^n$ value the latter is substituted in the equation (1) and equation is solved by iteration method to obtain f_0^{n+1} function. When the relative change of f_0 in all grid points, is less than given parameter ε the iteration procedure will stopped, i.e. [11]

$$|f_0^{m+1} - f_0^m|/f_0^m < \varepsilon \quad (3)$$

where m is the second internal circle iteration number. In the code the number of iterations is restricted by the value $M_{\max}$. Using obtained value of f_0^{n+1} the term $(dn_e/dt)^{n+1}$ is calculated and the calculation procedure is repeated. The iteration process is ended when criterion [11]

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$$[(dn_e/dt)^{n+1} - (dn_e/dt)^n]/(dn_e/dt)^n < 0.001 \quad (4)$$

is satisfied and function f_0^{n+1} is considered as a look for solution. After the distribution function was found various characteristics of plasma are calculated. In this paper we applied steady state electric field hence, the set of the characteristics are

The mean electron energy

$$\bar{u} = \int_0^\infty u^{3/2} f_0(u) du \quad (5)$$

The mean electron temperature

$$T_e = \frac{1}{k_B}\frac{2}{3}\bar{u} = \frac{1}{k_B}\frac{2}{3}\int_0^\infty u^{3/2} f_0(u) du \quad (6)$$

The rate constants

$$k = \sqrt{\frac{2}{m}} \int_0^\infty uQ(u)\, f_0(u) du \quad (7)$$

The electron mobility μ_e is defined by the ratio of the drift velocity W_e of charged particle and electric field E. It is given by

$$\mu_e = -\frac{1}{3}\frac{2e}{m}\int_0^\infty \frac{u^{3/2}}{v_m(u)}\frac{\partial f_0}{\partial u} du \quad (8)$$

where v_m represent the electron momentum- transfer collision frequency. So the drift velocity is

$$W_e = -\frac{E}{3}\frac{2e}{m}\int_0^\infty \frac{u^{3/2}}{v_m(u)}\frac{\partial f_0}{\partial u} du \quad (9)$$

The relation between electron diffusion coefficient and electron energy distribution function is given by

$$D_e = \frac{1}{3}\frac{2}{m}\int_0^\infty \frac{u^{3/2}}{v_m(u)} f_0 du \quad (10)$$

Characteristics energy gives by relation

$$\mu_{\text{ch}} = e\frac{D_e}{\mu_e} \quad (11)$$

2. Results and Discussions

The influence of the electron distribution function (EEDF) vs. the mean electron energy for different ratio of electric field to the gas density (*E*/*N*) in mentioned mixture is shown in figure (1). Clearly, the electron energy distribution function is strongly affected by changing the parameter

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E/*N*, subsequently the electron transport coefficients depends on the ratio *E*/*N*. The EEDFs profiles of the mixture with various *E*/*N* have several distinguished curvatures for all electron energies used. Close to the thresholds of the inelastic processes, the formation of the EEDF is strongly influenced by the electric field, which heats the electron component and thus increases the energy of the cold electrons. It is obviously appears from the figure that applying a high electric field (or *E*/*N*) leads to the development of EEDF to a higher energy tail.

The resulting shapes of EEDF in figure (1) at various *E*/*N* are significantly affected by increasing the mean electron energy. It can be observed that the mean electron energy for constant value of electron density is increases with increasing reduced field strength to *E*/*N*. The numerical result shown in figure (2) is in well agreement with this recognized knowledge.

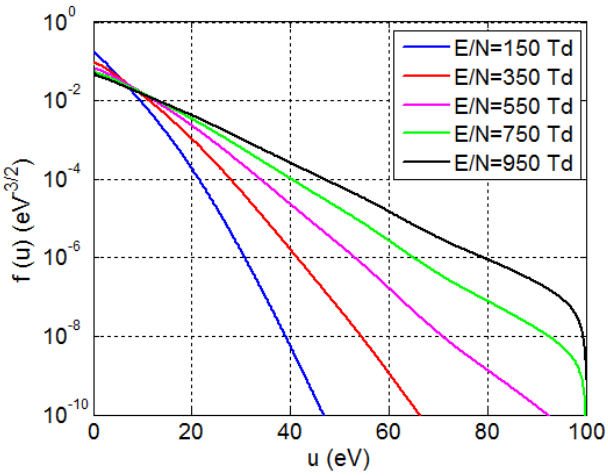

Figure (1)

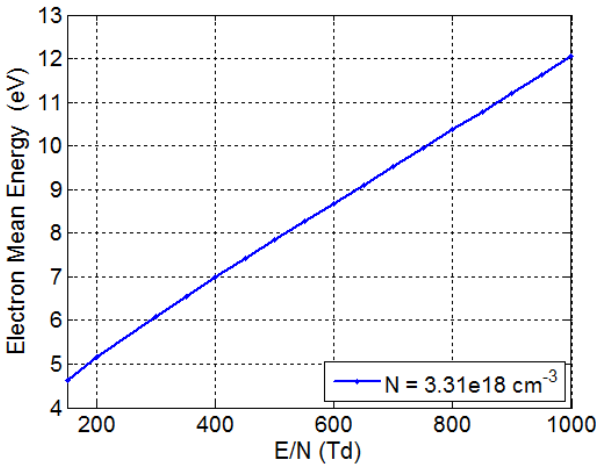

Figure (2)

Figure 1: EEDF for various values of reduced electric fields *E/N* (Td) vs. mean electron energy in mixture of (50% SF_6 – 50% Xe), the electron concentration is 3.31×10^{18} cm^{-3}, the temperature is 273 ^{0}K, and the pressure is 760 torr.

Figure 2: Calculated mean electron energy as a function of reduced electric field *E/N* in mixture of (50% SF_6 – 50% Xe) the electron concentration is 3.31×10^{18} cm^{-3}, the temperature is 273 ^{0}K, and the pressure is 760 torr.

The characteristic energy for the mentioned mixture vs. *E*/*N* is shows in figure (3). The characteristic energy increases gradually as *E*/*N* increased. However, the relation between them in the lower *E*/*N* < 400 Td is not linear.

Figure (4) expresses the dependence of electron diffusion coefficient with *E*/*N*. As *E*/*N* increases the electron diffusion coefficient slowly increased until the dependence becomes linear.

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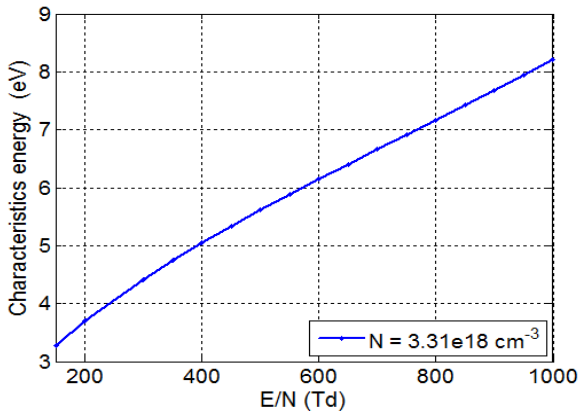

Figure (3)

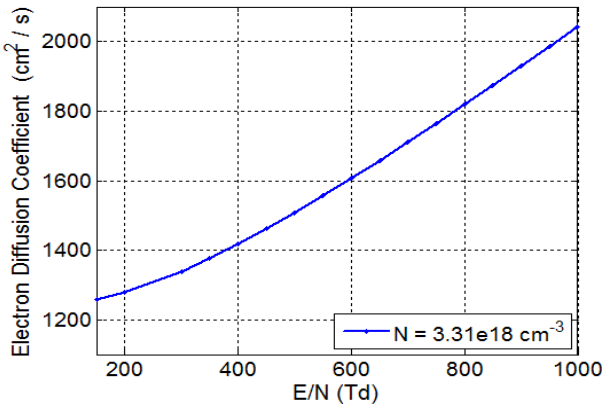

Figure (4)

Figure 3: Characteristic energy as a function of *E/N* in mixture of (50% SF_6 – 50% Xe), the electron concentration is 3.31×10^{18} cm^{-3}, the temperature is 273 ^{0}K, and the pressure is 760 torr.

Figure 4: Electron diffusion coefficient as a function of *E/N* in mixture of (50% SF_6 – 50% Xe) the electron concentration is 3.31×10^{18} cm^{-3}, the temperature is 273 ^{0}K, and the pressure is 760 torr.

The molecules in neutral gases have velocities in random directions. Under the action of an electric field *E*, positive ions move parallel and electrons anti-parallel to the direction of *E*, acquiring a drift velocity. The drift velocity has a direct linear dependence on *E*/*N* as shown in figure (5).

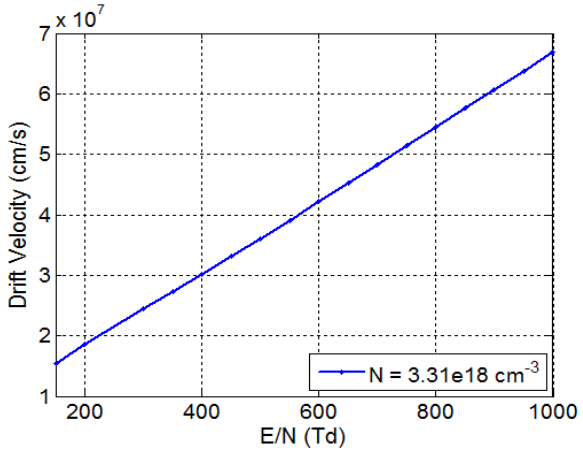

Figure (5)

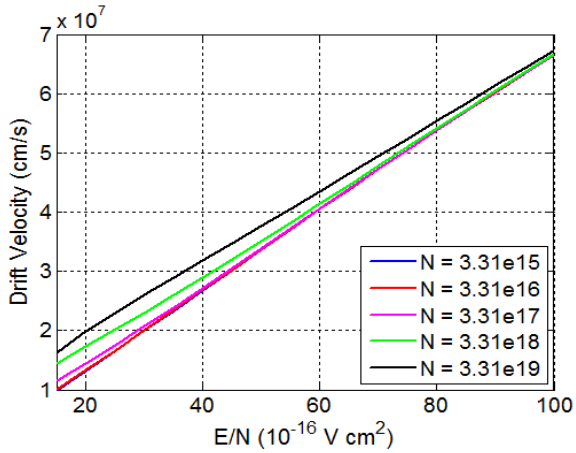

Figure (6)

Figure 5: Drift velocity as a function of reduced electric field *E/N* in mixture of (50% SF_6 – 50% Xe), the electron concentration is 3.31×10^{18} cm^{-3}, the temperature is 273 ^{0}K, and the pressure is 760 torr.

Figure 6: The variation of drift velocity as a function *E/N* in mixture of (50% SF_6 – 50% Xe), for various values of the electron concentration, the temperature is 273 ^{0}K, and the pressure is 760 torr.

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The classical theory of the electron drift in gases describes the electron drift velocity as universal function of *E*/*N*. The same drift velocity should be found at constant *E*/*N*. This is true for the gas below the atmospheric pressure. Even all the curves in figure (6) show the same behavior; that is as the electron concentration increased the drift velocity become higher with constant *E*/*N*. This can be distinguish at lower *E*/*N*, while the curves of become closer at higher *E*/*N* indicating small effect. The drift velocity is a linear function with *E*, and the mobility depends on strength field. At sufficiently low *E*/*N*, where an electron loses all equal to the gain from the electric field at one elastic collision, the drift velocity is proportional to *E*/*N*.

There is a different in electron transport coefficients between atomic gas (Xe) and in molecular gas (SF_6). In the former an elastic collision of electrons with atoms occurs, while in the latter electrons collisions with molecules occur as both elastic and inelastic processes. Hence, a small amount of molecular addition changes strongly the electron transport coefficients in mixtures. Figure (7) shows the variation of mean electron energy vs. *E*/*N* for different electron concentration. The higher the electron concentration is the lower curve of mean electron energy. The curves evidently split in lower *E*/*N* and become convergent at higher *E*/*N*. The reason of can be attributed to the variation of EEDF for different electron concentration.

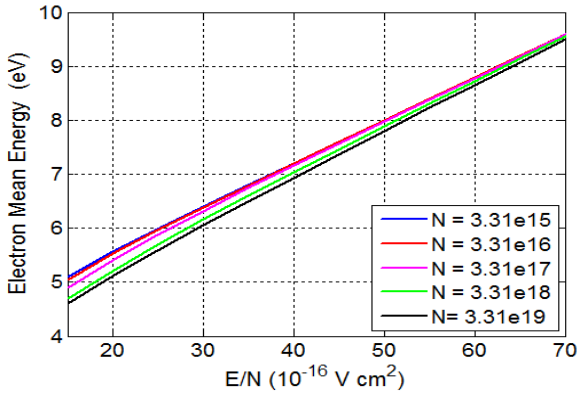

Figure (7)

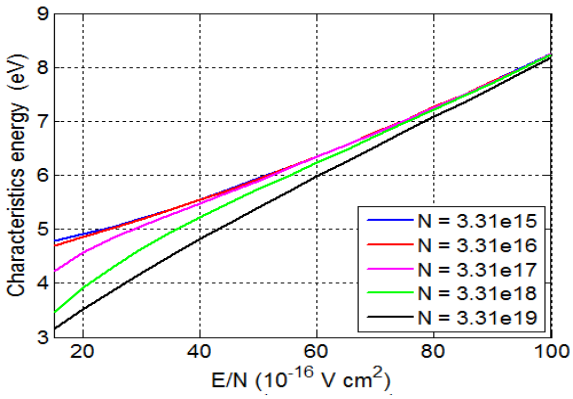

Figure (8)

Figure 7: The variation of mean electron energy as a function *E/N* in mixture of (50% SF_6 – 50% Xe), for various values of the electron concentration, the temperature is 273 ^{0}K, and the pressure is 760 torr.

Figure 8: The variation of characteristic energy as a function *E/N* in mixture of (50% SF_6 – 50% Xe), for various values of the electron concentration, the temperature is 273 ^{0}K, and the pressure is 760 torr.

Figure (8) denotes the variation of characteristic energy vs. *E*/*N* for different electron concentration. At lower *E*/*N* the curves of the characteristic energy are distinct and separated from each other while they are converge at the higher value of *E*/*N*.

Figure (9) shows the electron mobility with *E*/*N* for various values of electron concentration. The electron mobility is inversely exponential proportional with *E*/*N* since the electron energy loss result through the collisions between electrons and neutral molecules. The higher electron concentration gives upper curve for this relation. At high *E*/*N* the curves are converge closely from each other.

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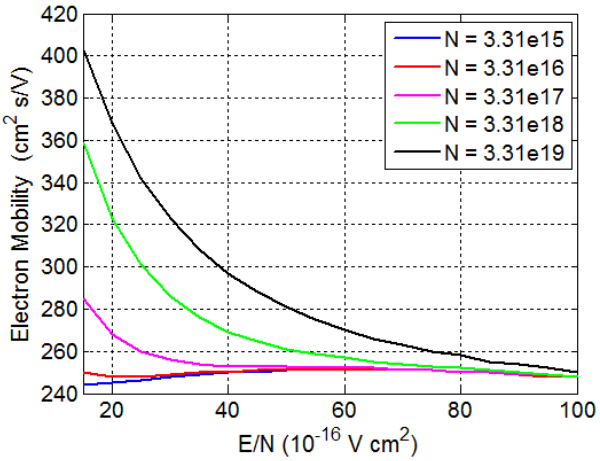

Figure (9)

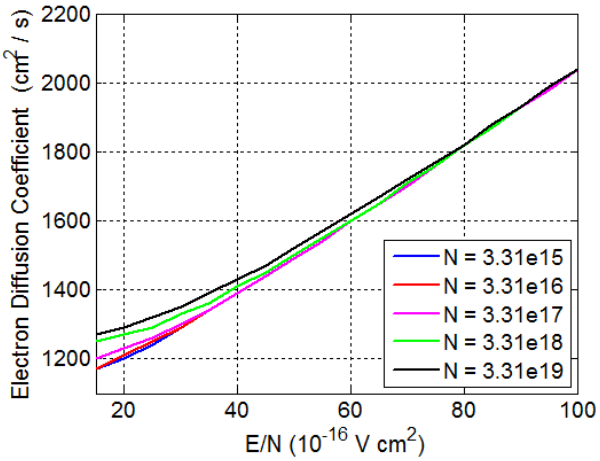

Figure (10)

Figure 9: The variation of electron mobility as a function *E/N* in mixture of (50% SF_6 – 50% Xe), for various values of the electron concentration, the temperature is 273 ^{0}K, and the pressure is 760 torr.

Figure 10: The variation of electron diffusion coefficient as a function *E/N* in mixture of (50% SF_6 – 50% Xe), for various values of the electron concentration, the temperature is 273 ^{0}K, and the pressure is 760 torr.

Figure (10) expresses the dependence of electron diffusion coefficient with *E*/*N* for various values of electron concentration. As *E*/*N* increases the electron diffusion coefficient gradually increased from exponential to linear form and converges very closely at higher *E*/*N*.

3. Conclusions

Solving Boltzmann equation using EEDF software package program over the range $150 < E/N < 1000\,Td$ ($1\ \mathrm{Td} = 10^{-16}\ \mathrm{V\,cm^2}$), where E is a uniform electric field and N is the gas density of the mixture, at temperature 300 ^{0}K and pressure 760 Torr are achieved. We show the influence of changing the electron concentration in a mixture of (50% SF_6 – 50% Xe) on the EEDF and the correspondent electrons transport. The important of such calculations relay on its direct usage in electrical discharge engineering. This work achieves and investigates previous work, whether it is theoretical or experimental and is compatible with them.

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