Simulation of Electron Swarm Parameters in CO_2, Xe and their mixtures using Boltzmann Equation

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محاكاة معاملات حشد الألكترون في الغازين ثاني اوكسيد الكربون و الزينون مع خليطيهما باستخدام معادلة بولتزمان

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الخلاصة

استخدم معادلة الأنتقال الطاقي لبولتزمان لحساب دالة توزيع طاقة الألكترون و معاملات الأنتقال في الغازين (CO_2، Xe) و خليطيهما. و تم تقدير معاملات حشد الألكترون ضمن المدى ($1\times10^{-18} \le E/N \le 2\times10^{-15}$) فولت.سم^2. ومن هذه المعاملات: سرعة الأنجراف و معامل التأين كدالة لنسبة شدة المجال الكهربائي الى الكثافة العددية للغازات. تم استخدام بيانات المقاطع العرضية المعتمدة على طاقة للألكترون. لقد وجد بأن دوال التوزيع هي لاماكسويلية و تمتلك اختلافات في الطاقة تعكس دور عمليات تبادل طاقة الأكترون الجزيئي.

Abstract

The Boltzmann transport equation is used to calculate the electron energy distribution function (EEDF) and the transport parameters in pure CO_2, Xe and their mixtures. Moreover, the electron swarm parameters are evaluated in the rang $(1\times10^{-18} \le E/N \le 2\times10^{-15})$V.cm^2. These parameters, namely are drift velocity and ionization coefficient. Reported electron cross-section data have been used in the calculation. The calculated distribution function are found to be remarkably non-Maxwillian that have energy variations which reflect the import electron-molecule energy exchange processes the importance of the results obtained from molecular gas discharge lasers is also discussed.

Keyword: Swarm parameters, Kinetic and transport theory of gases, Plasma and electron discharges, Electric phenomena in gases, Laser physics.

Theory

1-Boltzmann equation

The Boltzmann equation is the equation of continuity for electrons in a six-dimensional phase space and describe the time evolution of the electron energy distribution function $f(r,v,t)$. Electron transport and excitation coefficients are calculate as average of integral involving *f*. The electron energy distribution function contains all the information about the electron swarm and the calculated swarm parameters are average in the same sense that the experiments measure average quantities. The Boltzmann equation maybe written as [1]:

$$\frac{\partial f}{\partial t} + V.\nabla_r f - a \bullet \nabla_V f = C(f) \ldots\ldots\ldots\ldots (1)$$

Where *a* is the acceleration due to the applied field, and *C* is the collision operator. If the momentum transfer rate is large compared to the collision energy rate, a two–term expansion of the velocity distribution in spherical harmonic will be sufficient .This condition is found in atomic gasses and metal vapor at lower *E/N* . The numerical solution of Boltzmann's equation begins to fail at values of *E/N* greater than about *500Td* (where $1Td=10^{-17}V/cm$). This occurs as the drift velocity becomes non-negligible compared to the thermal velocity, violating the assumptions underlying the two-term spherical harmonic expansion of Boltzmann's equation [2].

2-Transport parameters

When the swarm parameters for each of the component gases in the mixture known, the values of the parameters in the mixture used to be evaluate by assuming a linear relationship between these values and the partial pressure ratios of the mixed component gases. This method may be only valid when the electron collision cross sections of the component gases are so similar to each other that the electron energy distribution is not so much modifies by mixing these gases [3].

Electron swarm motion, when the electric field is in the Z-direction, is represented by the following transport equation which monitors how the electron number density *n(r,t)* varies in time and space[4]:

$$\frac{\delta n}{\delta t} = D\left(\frac{\delta^2 n}{\delta x^2} + \frac{\delta^2 n}{\delta y^2}\right) - V_d \frac{\delta\ n}{\delta z} + D\frac{\delta^2 n}{\delta z^2} \ldots . (2)$$

Where *D* is the Diffusion Coefficient.

The swarm parameters are defined in the term of the collision cross-section *Q* and the electron energy distribution function $f_o(u)$ as follows[1].

The drift velocity V_d, is:

$$V_d = -\left(\frac{2e}{m}\right)^{1/2}\left(\frac{E/N}{3}\right)\int_0^{\infty}\frac{u}{\sum \delta_S Q_{sm}(u)}\frac{df_o}{du}du \quad \ldots..(3)$$

Where u is the electron energy in (eV).

δ_S is the number density of molecules of species S divided by gas number density N ($\delta_S = \frac{N_S}{N}$), $Q_{sm}(u)$ is the momentum transfer cross-section for elastic collisions of electron with energy u with molecules of species S.

The ionization coefficient is [5]:

$$\frac{\alpha}{N} = \frac{1}{V_d}\int_0^{\infty} Q_i(u)\left(\frac{2e}{m}\right)^{1/2} f(u)du \quad \ldots\ldots(4)$$

Where $Q_i(u)$ is the ionization cross-section.

The cross-section

1- Carbon dioxide

Current interest in carbon dioxide is high due to its use in high power lasers, usually as a mixture constituent. Work directed toward understanding laser mixtures has frequently included data for pure CO_2 [1].

A set of cross-section representing electron collisions in carbon dioxide are given. The momentum transfer (elastic collision) cross-section is given too [6].

Four types of inelastic cross-section have considered.

The vibration cross-section has been divided into four main vibration levels as given by [5] with onset energies *(0.0827, 0.291, 0.580 and 0.870)eV*. The total ionization cross-section having onset energies of *13.3eV* is given by Itikawa and Mason[7]. Excitation cross-section is given by [6].

2- Xenon

For Xe atom, the electron-impact cross section for momentum transfer, Q_m is taken from the data of [8], and the total ionization cross-section Q_i, from the ground state employed using the experimentally determined value of [7].

Result and Discussion

The distribution function is defined such that $\int_0^\infty u^{1/2} f(u)du = 1$ clearly, the calculated distribution function are markedly non-Maxwillian, having energy variations which reflect the dominant electron-Molecule energy exchange processes as in figure (1&2). In figure (1) at lower energy $E/N = 1\times10^{-19}\ V.cm^2$, the normalized distribution appears to be quite close to a straight line with hence quite close to the Maxwillian distribution. However, for high *E/N* value ($1\times10^{-15}V.cm^2$) the distribution is non-Maxwillian.

In figure (2), the vibrational energy losses in CO_2 are distributed more energy and therefore, structure in $f(u)$ is less apparent. Never the less, the dip in $f(u)$ near 1eV can be identified with electron energy loss to the asymmetric stretch vibration in CO_2 for which the cross section is relatively large in this energy range. The influence of different discharge parameter on the electron distribution function of Xe and CO_2 (50:50) gas mixtures are demon started in figure (3), for *E/N* values typical of CO_2 laser discharges $E/N = 3\times10^{-16}V.cm^2$ exhibit the distinctly portions that have been determined The electron energies are thermal and the energy distribution is Maxwellian in which represent by a straight line variation .However for $E/N = 3\times10^{-16}V.cm^2$ the distribution is Clearly non-Maxwellian.

With a know ledges of the electron energy distribution function it is possible to perform an energy balance by integrating the electron kinetic equation over all electron energies.

The most computed swarm data are the drift velocity and ionization coefficient. Throughout the range of *E/N* value the electron drift velocity V_d calculation for pure Xe and CO_2 have been made down as shown in figures (4 & 5) using equation (3), in order to overlap with the values calculated from Boltzmann equation.

Electron in an ordinary case, have an ordinary movement that is define as thermal motion, but with increasing *E/N* value. The speed of electrons will increase too; this will lead to another kind of motion known as the drift motion. Figure (4) is representing the drift velocity of pure Xenon as a function of *E/N*. the drift controlled by inelastic collisions. The drift velocity is proportional to *E/N*, and it takes higher value with increasing of *E/N*, since the elastic scattering cross section decreases strongly with the energy in this range of *E/N*.

As we seen in this figure, *E/N* increases rapidly for wide E/N rang ($1\times10^{-19} \le E/N \le 6\times10^{-19}$) V.cm^2, which is due to the reduction of the number of collisions as the energy of the swarm coincides with the sharply decreasing part of momentum transfer cross section Q_m.

The gradient of V_d should be larger than else where, on the other hands the energy moves on the increasing parts of Q_m the slop of drift velocity will be much smaller. The drift velocity calculations in figure (5) have made in order to overlap with the values calculated from Boltzmann equation. The computations are very sensitive to the magnitude and shape of the variation cross-sections.

Figure (6) is representing the drift velocity for CO_2-Xe (10:90) mixture ratio. The ionization energy of Xe=*12.13eV* while for CO_2=*13.3eV*.

Although, the ionization energy of Xe is lower than that of CO_2, when the ionization process begins, the free path of Xe is shorter than that of CO_2, then the acceleration path of Xe is shorter than that of CO_2 and thus the accumulation collision energy is lower than that of CO_2, on the other hand the molecular weight of Xe is grater than that of CO_2.[Xe=131.3, CO_2=44.009].

Thus, after the electron collision process with Xe molecules starts, the electron drift velocity decreases more quickly, and the number of high energy electrons reduces further than that with CO_2.

The Townsend ionization coefficient *α/N* has been calculated in figure (7) using equation (4) for rang ($4\times10^{-17} \le E/N \le 2\times10^{-15}$). The results are shown The behavior of ionization coefficient which increases with increasing of *E/N* The result of high *E/N* are sensitive to the inelastic collision .this means that the electrons acquire enough energy from the applied electric field to reach the ionization level of Xe, In this case, the number of energetic electrons, which cause the ionization, increases with increasing *E/N* according to the ionization cross sections of Xe. And also in figure (8) the agreement is very good over the entire *E/N* range, it agrees with the data of Bhalla and Cragges [9].

At low *E/N* only a small shift in mean energy is necessary to give exact agreement. The increase in mean energy causes an increasing in *α/N*.

Conclusion

The behavior of electron swarms in gases has been studied employing a Boltzmann equation; calculations for electron energy distribution function for electric discharges in CO_2, Xe and their mixtures containing these species have showed that the distribution function is highly non-Maxwillian.

The first asymmetry term in the expansion of the EDF in spherical harmonics was as high as of the symmetric part of the distribution function; on the other hand, the determination of the Townsend ionization coefficient or other collision rates requires knowledge of the EDF above the ionization potential.

The results have shown that the calculated swarm parameters, which are the electron-drift velocity and ionization coefficient for pure CO_2, Xe and their mixtures were in good agreement with computational works.

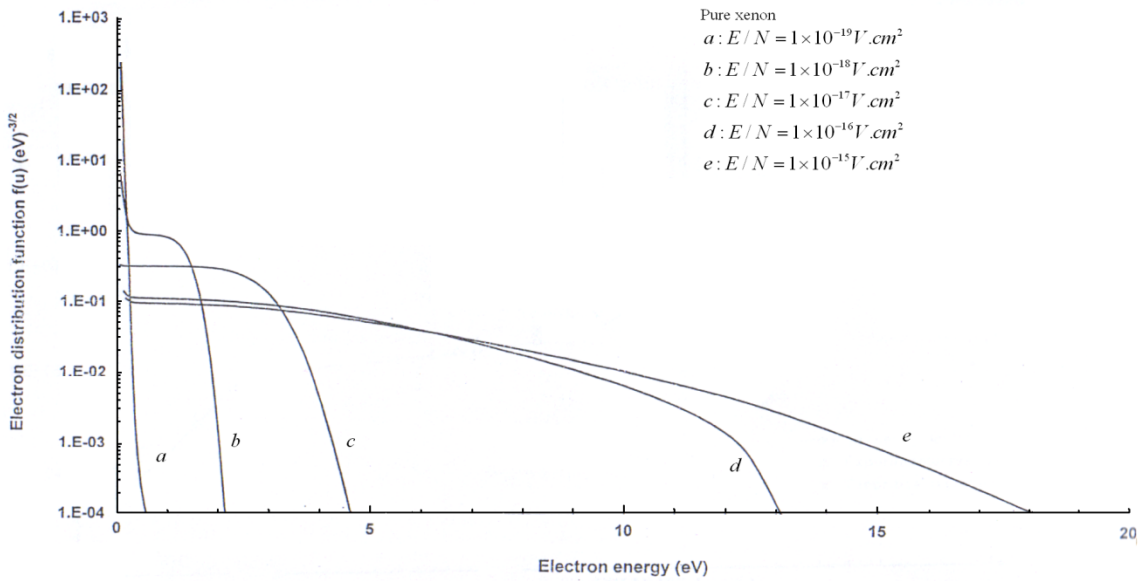

Figure 1: The electron energy distribution function in pure xenon gas for several values of E/N.

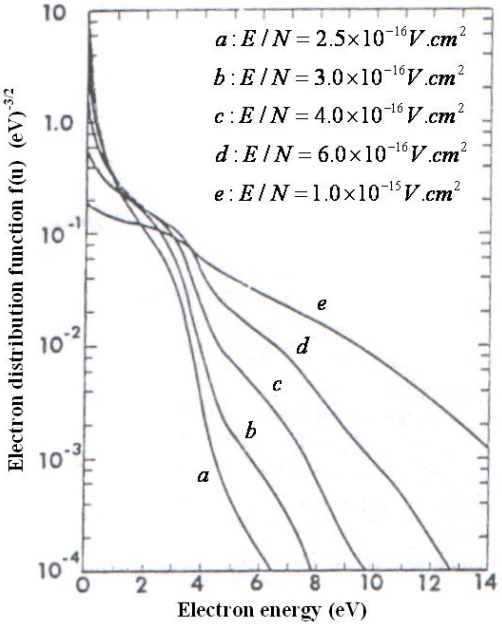

Figure 2: The electron energy distribution function in pure Carbon dioxide as a function of *E/N* for several values of *E/N*.

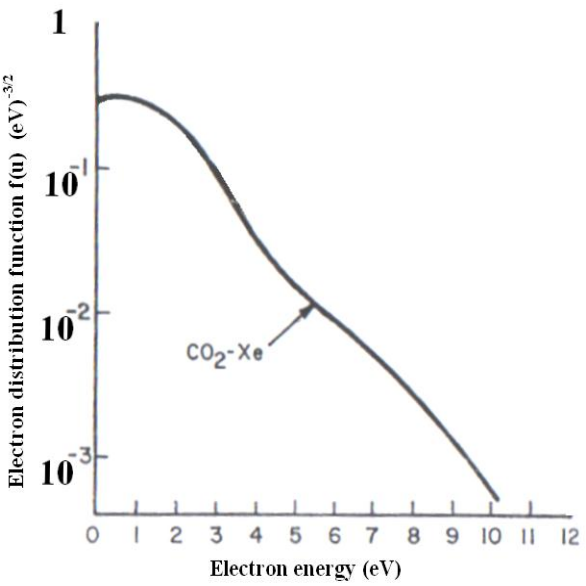

Figure 3: The electron energy distribution function as a function of electron energy in CO_2:Xe gas mixtures (50:50) at *E/N*= $3\times10^{-16} V.cm^2$.

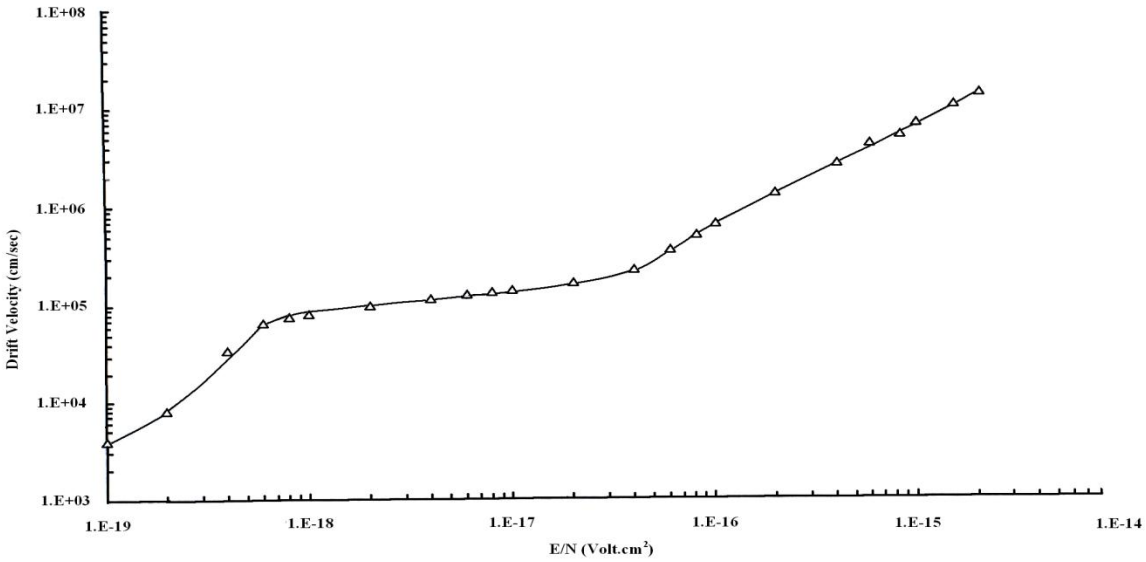

Figure 4: The drift velocity of electron as a function of *E/N* for pure xenon gas.

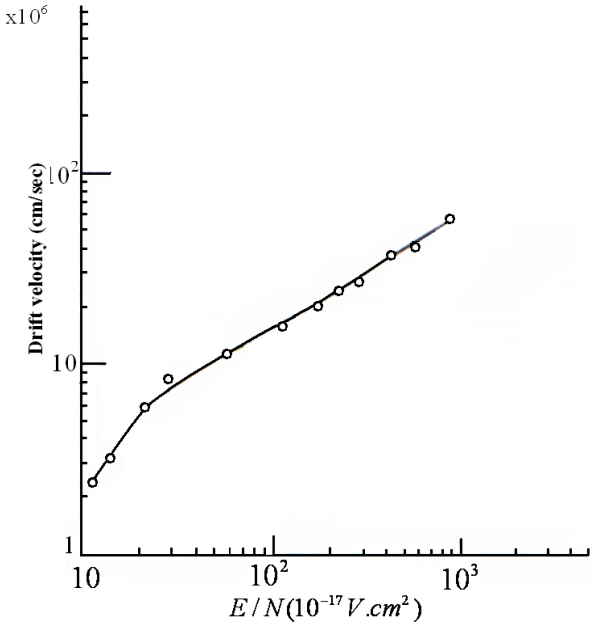

Figure 5: The drift velocity as a function of *E/N* for Carbon dioxide.

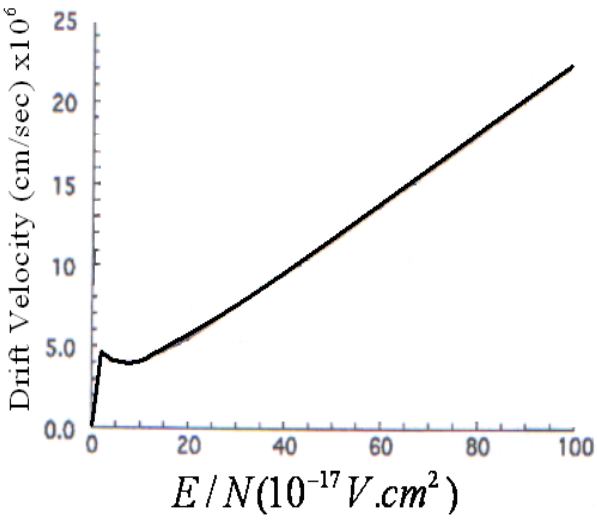

Figure 6: The drift velocity as a function of *E/N* for CO_2-Xe (10:90).

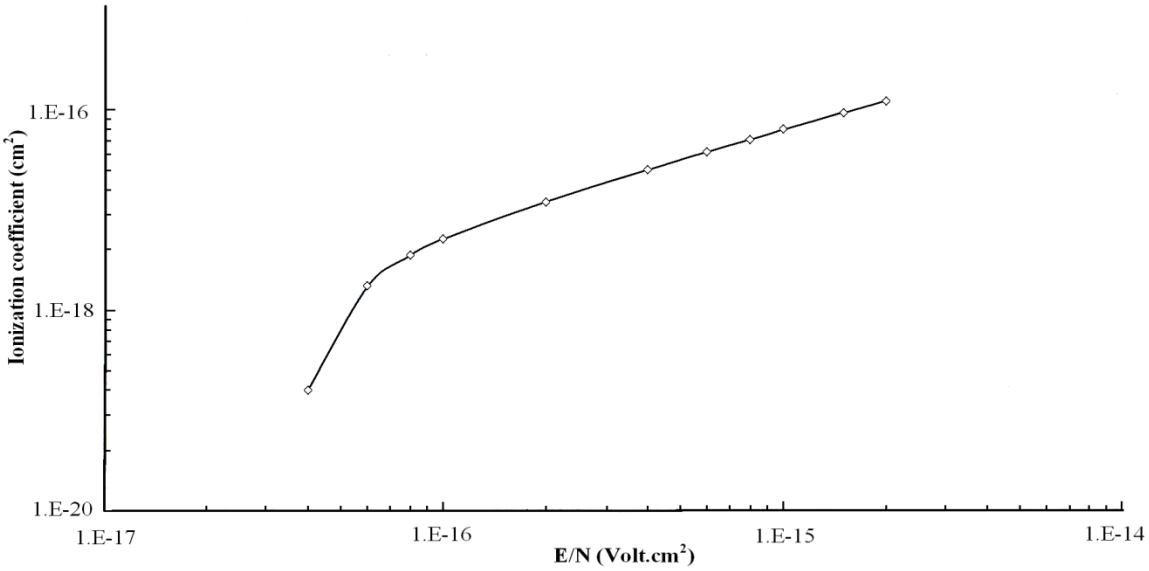

Figure 7: The ionization coefficient of electrons as a function of *E/N* for pure Xenon gas.

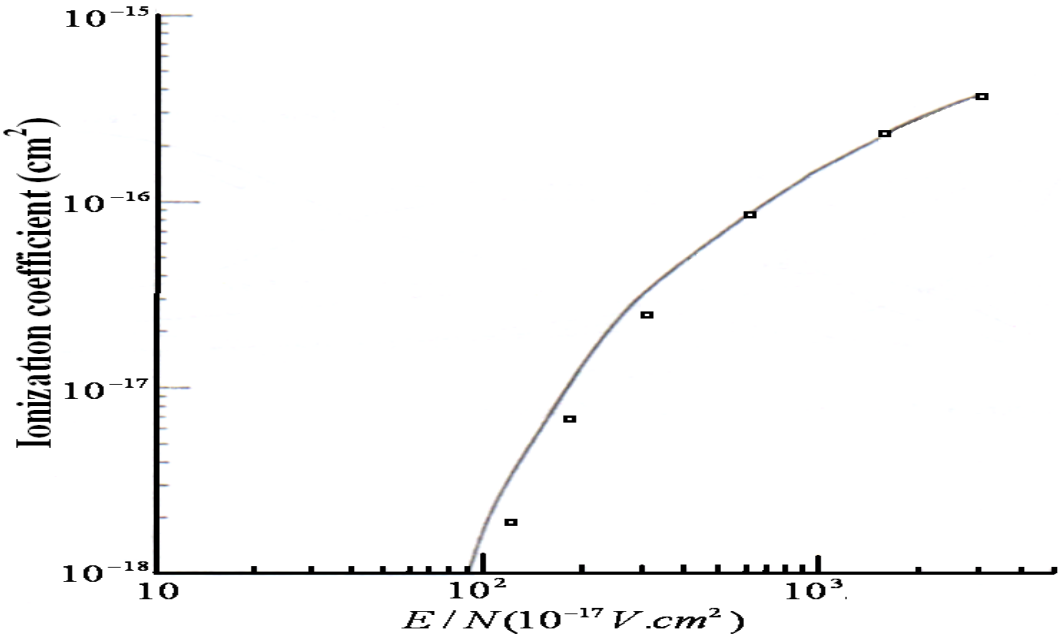

Figure 8: The ionization coefficient of electrons as a function for *E/N* in Carbon Dioxide.

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