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Study on the Effect of H_2 Addition to N_2 on EEDF and Electron Transport Coefficients

Mustafa. K. Jassim
Department of Physics, College of Education for Pure Science, Ibn Al – Haitham, University of Baghdad.
qqqqq1961@gmail.com

Enas A. Jawad
Department of Physics, College of Education for Pure Science, Ibn Al – Haitham, University of Baghdad.

Jamal K. Alsaide
Ministry of Science and Technology, Baghdad.

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Abstract

In this paper, we calculate the electron energy distribution function (EEDF) and transport parameters including the electron mean energy, mobility, drift velocity and diffusion coefficient for the gas mixtures of the H_2 and N_2 using the EEDF program. It is concentrated on the effect of assorted concentrations of the mixtures on the EEDF and the electron transport coefficients. The work exhibits the variation amongst the different mixtures on the EEDF and the transport parameter. The results are graphically offered and discussed. In this concept, it is shown that for each mixture has a specific impact on EEDF and the transport parameter. The important of this study comes from the usage of these mixtures in DC (direct current) glow discharge. These results are salutary to detect the best gas mixtures to reach proper transport parameters.

Keywords: (EEDF) program, EEDF, Boltzmann equation, H2, N2, transport coefficients.

1. Introduction

In plasma modelling the electron energy distribution function EEDF is needed to calculate the reaction rates for the reactions of electron collision [1,2]. The effect elastic collisions are governed on the EEDF, while the inelastic collisions are not important [2]. EEDF can be describe by the solution Boltzmann equation BE [3]. On the other hand, the physics of electron swarm parameters has been engaging enormous attention over the past decades because of the solicitude in many of the physical effects that occur in these settings and the need for accurate input data in discharge modelling. Numerical techniques and computer resources have made it possible to obtain more specifics about the physics of particle swarms. Most of the intent has been devoted to electron swarms, the function of the distribution of electronic energy and transport properties has been specified for a vast extent of gases and gas mixtures [4].With the aid of a program EEDF, we can be simulating the electron transport parameters in gas under influence of an electric field [5-10].The aim of this work is to investigate theoretically the electron energy distribution function and electron transport parameters in direct current (DC) electric discharge processes in H_2 and N_2 gases mixtures to different proportions. We calculate electron transport parameters of H_2 and N_2 gas mixture are executed under standard conditions 25 C^o and 760. The transport parameters are limited to a function of reduced electric field E/N for different rates of increase of the electric field [11].

2. Theory

It is Known that a particle moving around in the 3 dimensional space, the phase space basically consists of all points (x, y, z, P_x, P_y, P_z), where x, y, and z are the three directions in space, and P_x, P_y, and P are the momenta in the x, y, and z directions. So, the phase space of one particle has 6 mathematical dimensions. The electron equation of continuity $f\ (r, v, t)$ in a six-dimensional phase space that identify the time evolution for electron energy distribution function (EEDF) is known as Boltzmann equation (BE). This equation includes the whole information of the electron. By using two-term approximation for the distribution function, the code EEDF solve steady state BE in homogenous plasma for isotropic portion of the electron distribution function. The BE under regard is given by:

$$\sqrt{u} f_0(\varepsilon) \frac{dn_e}{dt} = I_E(\varepsilon) + I_{in}(\varepsilon) + I_{el}(\varepsilon) + I_{ee}(\varepsilon)$$

The BE picks into consideration the change of the electron density in the ionization, recombination and attachment processes. The term$f_0(\varepsilon)$is the isotropic portion of the distribution function, and$\varepsilon$is the electron energy. The terms $I_{ee}(\varepsilon)$,$I_E(\varepsilon)$ describe the electron-electron collisions and heating of electrons in the electric field, respectively. The other two terms $I_{el}(\varepsilon)$, $I_{in}(\varepsilon)$characterizeelastic, inelastic collisions. In solving BE the electron transport is calculated as an average of integral that encompasses f in parallel manner as to the experiments measure average quantities [12]. Having known the transport parameters of each gas, we look at the transport parameters of the gas mixtures. The transport parameters of each mixture depend on the percentage of each gas in the mixture as well as the electron collision cross sections of the individual gas. Obviously, these two factors indeed modify the parameters of the transport of the mixture.

The mean electron energy is defined in term of distribution function $f_0(\varepsilon)$as:

$$\bar{\varepsilon} = \int_0^\infty \varepsilon^{3/2} f_0 d\varepsilon \ ,$$

And the mean electron temperature is:

$$T_e = \frac{2}{3K_B} \bar{\varepsilon} \ ,$$

The electron drift velocity is:

$$v_d = E\mu_e$$

where μ_e is the electron mobility given by:

$$\mu_e = -\frac{2e}{3m} \int_0^\infty \frac{\varepsilon^{3/2}}{\nu_m(\varepsilon)} \frac{\partial f_0}{\partial \varepsilon} d\varepsilon$$

The characteristic energy is given by:

$$\varepsilon_{ch} = e\frac{D_e}{\mu_e}$$

where D_e is electron diffusion coefficient given:

$$D_e = -\frac{2}{3m}\int_0^\infty \frac{\varepsilon^{3/2}}{\nu_m(\varepsilon)} f_0 d\varepsilon$$

In which the $\nu_m(\varepsilon)$ is the momentum transfer frequency:

3. Results and discussion

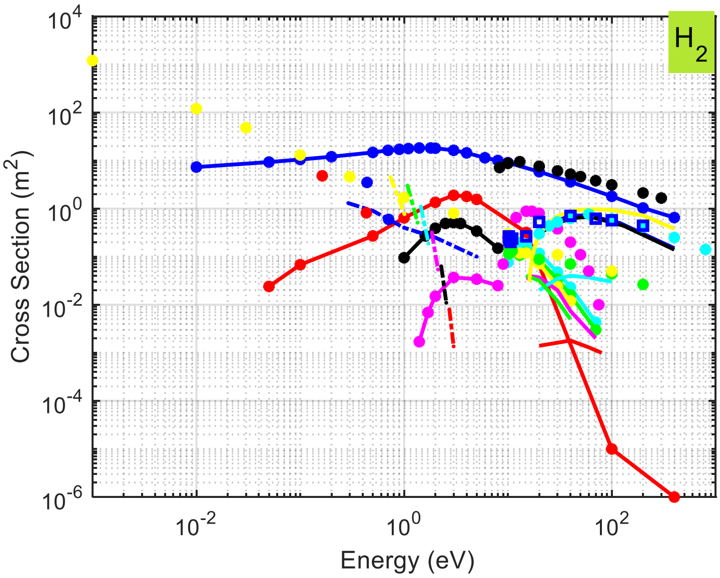

Figure 1. The cross sections of pure H_2 versus energy used in the calculations.

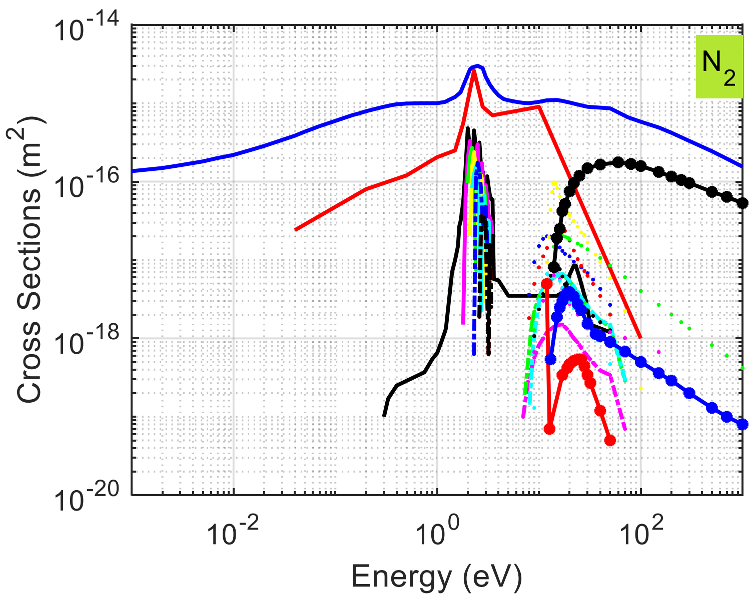

Figure 2. The cross sections of pure N_2 versus energy used in the calculations.

The cross section means the probability of two particles to react in some specific way. In order for the two particles to scatter from each other, their mutual cross section defined as the area that transverse to their motion within which they should meet. The cross sections are measured in units of area. It is important to have accurate absolute cross section to understand the conceptual of the electron collisions and the related plasma physics [13]. **Figures 1** and **2,** show the cross sections of both N_2 and H_2, respectively. The data is ready to use and visualize for each reactions of the gas. It is taken from sets of mentioned references in the program folder called GASFILES.

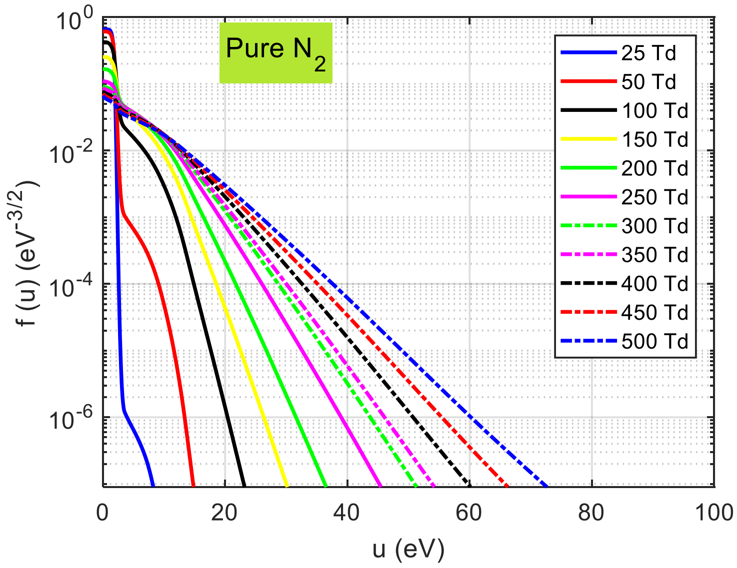

Figure 3. The electron energy distribution function of pure N_2 versus electron energy at different values of reduced electric field E/N.

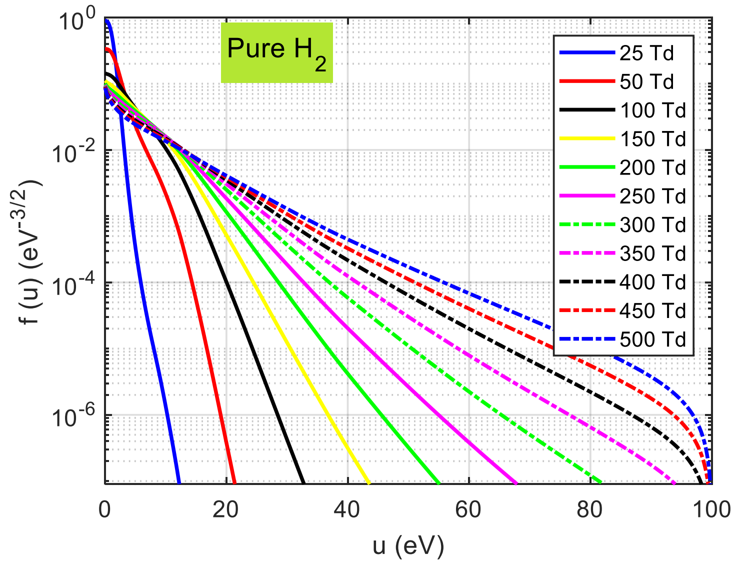

Figure 4. The electron energy distribution function of pure H_2 versus electron energy at different values of reduced electric field E/N.

Figures 3 and **4.** Show the electron energy distribution function as a function of electron energy at various values of reduced electric field E/N for pure N_2 and H_2, respectively. It is clear that distribution functions are significantly non-Maxwellian for whole E/N used, except for lower values that have lower energy. At these values, the straight line indicates that distribution has Maxwellian shape. As the E/N is increased the distribution functions located at higher energy range. Clearly, each curve of the distribution functions of similar value of E/N for both gases are different. The extension of the curves H_2 gas to a higher electron energy point out higher energy exchange between the molecule and electron at the same E/N compared to N_2 gas.

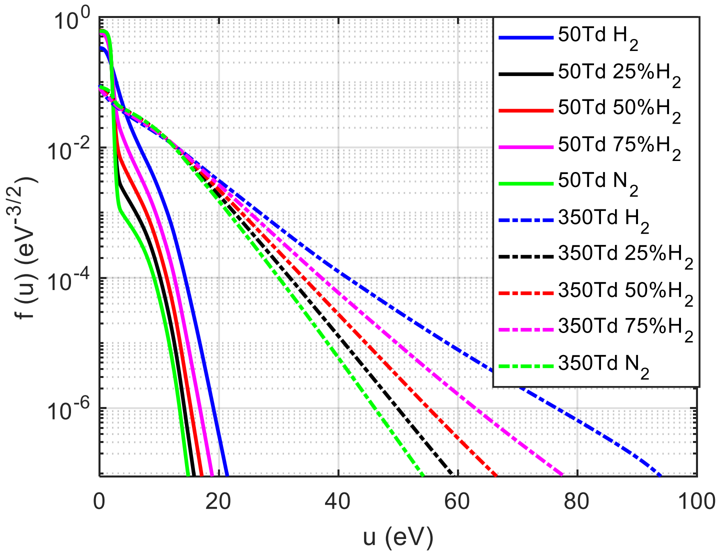

Figure 5. The distribution function of pure H_2 and N_2 and their mixtures versus electron energy at two different values of reduced electric field E/N.

Figure 5. Demonstrates the distribution functions as a function of electron energy for both gases and their mixtures at two values of E/N. The distribution functions for each gas identified according the own electron collision cross sections. The influence of mixture on the distribution function is shown by locating the profiles between the curves of pure two gases in a symmetric way. As the percentage concentration of N_2 increased in the mixture, the curve of distribution function is shifted towards the right. The presence of H_2 gas leads to more molecule-electron energy exchange extending the energy range. The shift of the mixture distribution function curves for constant E/N depend on the partial pressure of each gas and therefore, its electron collision cross sections which is modifies the electron energy distribution by mixing the two gases.

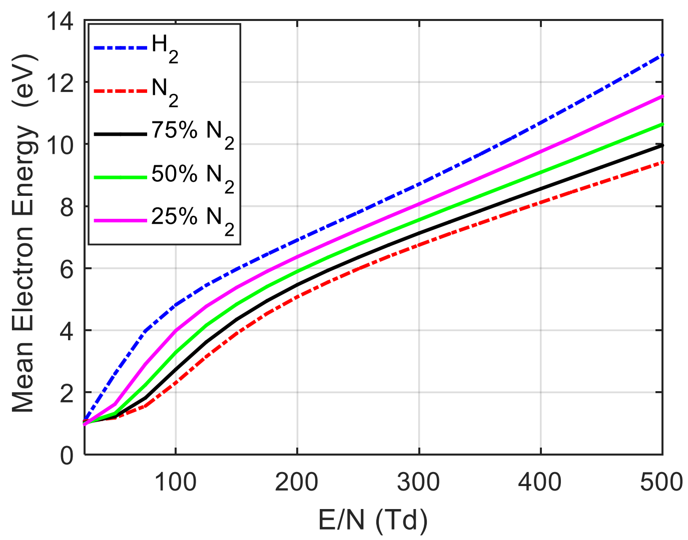

Figure 6. The mean electron energy as a function of E/N for pure H_2 and N_2 gases and their mixtures.

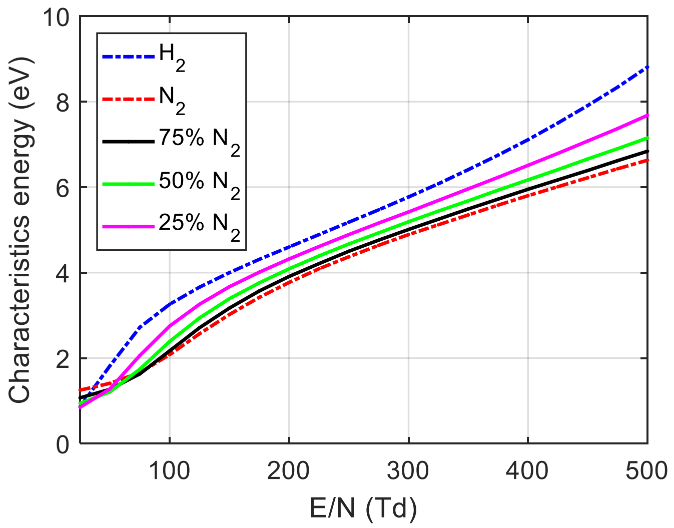

Figure 7. The characteristic energy as a function of E/N for pure H_2 and N_2 gases and their mixtures.

Figure 6. shows the variation of mean electron energy with E/N for pure H_2, N_2 and their mixtures. The behaviour of both pure gases is similar above E/N=100, however, at lower value than the mentioned, the increasing of the curves is different. The H_2 has curve grardually concave up increasingwhile the N_2 curve has expoenentially concave down increasing. The behviour of the mixtures depends on the percentage ratio of N_2 in the mix. The 50% concentration of N_2 is comprised between the curves of two purely gases. **Figure 7.** showsthe characteristic energy versus the E/N for the pure gases and their mixtures. Again, the curves have similar attitude. Despit of that the mixtures have higher values of chacteristic energy than the H_2 at exterimally lower vlues of E/N. Having known the curves of each compoenent of purely gases, one can expect the mixture curves. it is as if there is an upward shift by increasing the ratio of partial pressure of H_2 in the mixture, so it is possible to predict the reamain curves of other mixtures where it will be located.

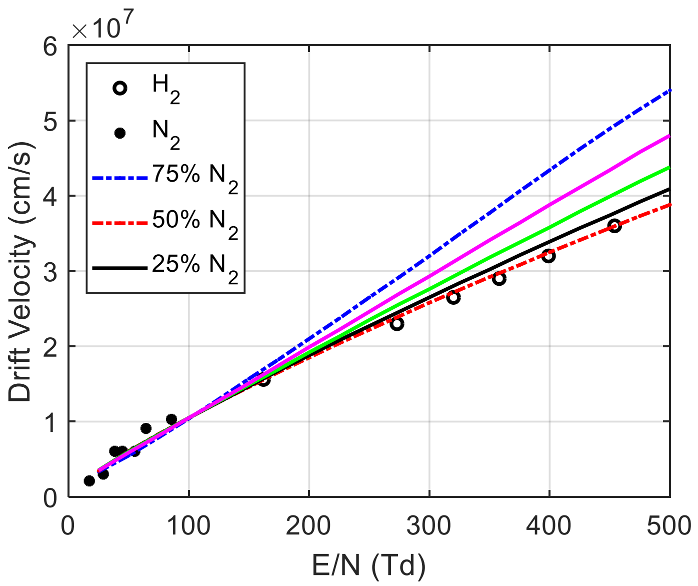

Figure 8. The drift velocity as a function of E/N for pure H_2 and N_2 gases and their mixtures.

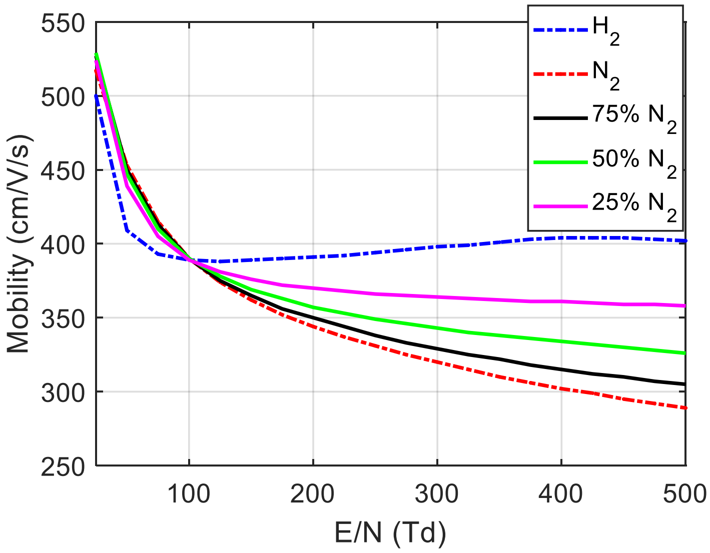

Figure 9. The mobility as a function of E/N for pure H_2 and N_2 gases and their mixtures.

The electron drift velocity in the electric field is the most important electron transport parameters that characterize the conductivity of a weakly ionized gas [14]. **Figure 8.** Shows the relationship between drift velocity and E/N for the H_2, N_2, and their mixture. In normal situation, the electron has movement due to the thermal motion; however, under increasing E/N the electron will have another type of movement; that is the drift velocity. The drift velocity is governed by the inelastic collisions. The calculations of drift velocity depend on the magnitude variation of the cross section and it shape. It is clear that the relationship between them is a linear for both the pure gases and its mixtures with different slopes due to strongly decreasing of elastic scattering cross section with the energy as E/N increased. The entire straight lines converge at E/N=100 Td and no effect of gases ratio appears. As explained before, the effect of percentage mixtures of the two gases appears in the location of the mixture curves in between the curves of the two pure gases. The role of percentage mixtures whether it is heavier or not in this point looks like to be negligible. The lower the percentage of N_2 gases in the mixture, the greater the slope of the mixture curve towards the H_2 curve. This effect is due decreasing of the molecular weight of N_2 that leads to increase the drift velocity. However, it is clear that the computations of electron drift velocity of N_2 and H_2 gases, as a function of reduced electric field, are consistent with experimental data [15,16]. **Figure 9.** Shows the dependence of mobility on the E/N for both two pure gases and their mixtures. The curves are exponentially decreasing with increasing E/N for pure N_2 and the mixture, while the curve of H_2 is linearly decreasing for the E/N values less than 100 Td and then gradually increases at higher E/N.

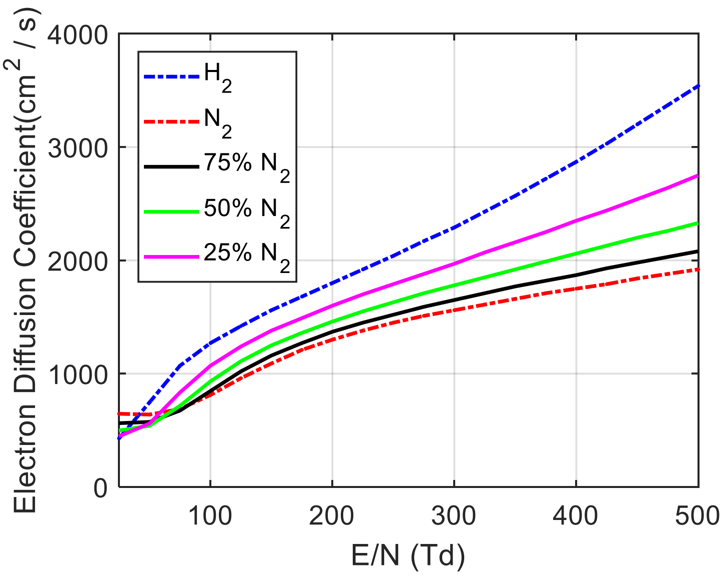

Figure 10. The electron diffusion coefficient as a function of E/N for pure H_2 and N_2 gases and their mixtures.

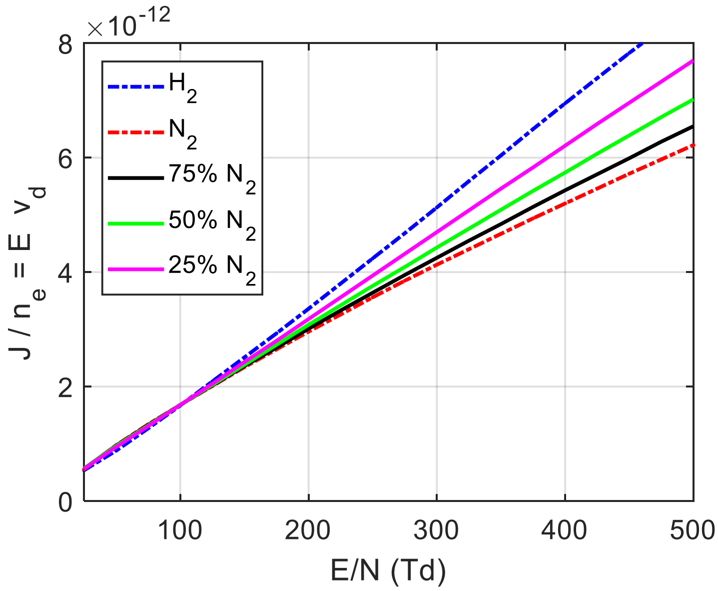

Figure 11. The $J/n_e = E\ v_d$ as a function of E/N for pure H_2 and N_2 gases and their mixtures.

Figures 10, 11. show the dependence of electron diffusion coefficient and $J/n_e = E\ v_d$ on the E/N for both two pure gases and their mixtures. A close glance to **Figures 7, 10.** One notices the symmetric behavior between the two graphs. Also, a similar description between the graphs of **Figures 4a, 6a.** The latter similarities come out due to multiplying the drift velocity by electric field.

4. Conclusion

Using EEDF program, electron energy distribution function and transport parameters as functions of reduced electric field have been theoretically performed for pure N_2, H_2 and their mixtures in order to assess the effect of nitrogen admixture in the gas. Prospectively the behavior of the transport parameters on the mixture percentage of the components, be elucidated by a discriminatory weighting of the elastic/inelastic scattering of the electrons on

N_2, H_2 molecules at different of E\N. Particularly, the whole calculated mixtures curves of both gases for plasma parameters are located between the extremely pure N_2, H_2 curves.

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