Studying the Swarm Parameters and Electron Transport Coefficients in N_2– CH_4 Mixtures Using BOLSIG+ Program

Haneen K. Ibrahim[1*], Enas A. Jawad[2], Mustafa K. Jassim[3]

Abstract

We have considered the electron transport coefficients and swarm parameters of pure nitrogen and methane gases and their mixtures for a large range of reduced electric field from 30 to 700 Td, using BOLSIG+ freeware. We inspect the relevant coefficients and parameters of pure methane and nitrogen that calculated in the program and visualized graphically. To analyze these data with other available data, we plot them collectively to find out the variation. This study and the data offered has a significance in plasma and space physics and many fields because methane is one of the greenhouse gases.

Key Words: Electron Swarm Parameters, Transport Coefficients, Methane, Nitrogen, BOLSIG+.

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Introduction

Various industrial and scientific applications requiring the electron transport coefficients and swarm parameters data in order to understand and anticipate the behavior of such applications [1, 2]. The coefficientsand parameters include mean electron energy, characteristic energy, mobility, drift velocity, diffusion coefficient, and the ionization coefficient. All of these depend on the electron energy distribution function (EEDF).To compute these data, it is customary to solve Boltzmann equation utilizing available electron cross sections of the gases. There are many of approaches with some physical and mathematical principles found to achieve the solution. One of them is the BOLSIG+ program, which is a freeware solver of Boltzmann equation that brings into account the fluid model of gas discharge [3].

For the electrons in a uniform electric field, the classical two-term expansion is applied in the program to obtain the steady state solutions.

Methane is one of the greenhouse gases that contributes significantly to global warming along the planet. It sets down into so many applications like plasma processing of semiconductor surfaces, particle counters, and control of pollution, and so on, placing human, beast and plant life in general at risk [4].The danger occurs from its extensive utilization in industrial applications [5].

Therefore, the world is moving towards developing contexts and treaties to cut down the use of these gases, according to international standards and protocols, and therefore must be adhered to in order to reduce the use of methane and its concentration in the atmosphere [6, 7]On the other hand, it is suitable to mix methane with other non-greenhouse gases to decrease its content in the gas mixture that is employed in such applications.

Corresponding author: Haneen K. Ibrahim

Address: [1*]Department of Physics, College of Education for Pure Science, Ibn Al – Haitham, University of Baghdad; [2]Department of Physics, College of Education for Pure Science, Ibn Al – Haitham, University of Baghdad; [3]Department of Physics, College of Education for Pure Science, Ibn Al – Haitham, University of Baghdad.

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Nitrogen gas is an alternative candidate for methane to enter industry and engineering applications because it is not a greenhouse gas due to its unique features as it is non-toxic in addition to its availability in the Earth's atmosphere[8, 9].Furthermore, due to its essential role in space research, such as some moons of the plants and the earth ionosphere, the data of electron transport and the swarm are important in the space research [10, 11].Hence known those data for the mixed gas help to understand related physical phenomena. In this context, Tezcan et.al[12] studied the swarm parameters such as electron mean energy, drift velocity, ionization coefficient, and effective ionization coefficient of the methane and nitrogen mixtures by solving the Boltzmann equation using a Townsend theory approach at steady state depending on the cross sections of these gases in the range between 80-400 Td of reduced electric field.

The purpose of this work is to expand the study to other parameters of methane and nitrogen mixtures, which were not addressed by Tezcan et.al[12], by using the freeware BOLSIG+ program to solve the Boltzmann equation that based on the fluid model. In addition, the range of the reduced electric field is expanded between 30-700 Td (1Td = 1 Townsend = 10^{-21} Vm^2). Therefore, this study will offer significant data on the electron swarm and transport parameters for methane-nitrogen mixtures, which are generally brief in scientific literature. The effects will likewise be compared with those available to view compatibility with them.

Brief Description of BOLSIG+ program

Since its release in 2005,BOLSIG+ program has become a widespread by the physicists of low temperature plasmas. It solves numerically the Boltzmann equation for electrons in weakly ionized gases and uniform electric fields and gas density, conditions that typically manifest in the extent of collisional plasmas with low temperature. The input considers complete cross sections sets of the gases. These sets, which are available directly in house selection of cross section of the gases, account in a regular way for the complete electron energy losses and momentum losses due to collisions. The program then provides output of EEDF, transport and rate coefficients, together with the swarm parameters verses reduced electric field from collision cross section data. It yields excellent accuracy and high calculation speed. All things considered of BOLSIG+ principles are firstly, the electric field is supposed to be uniform, and so the entire collision probabilities. Secondly, utilizing the classical expansion to approximate the angular dependence of the electron distribution. The third point is that the exponential growth model is considered for the variation of electron density because of the ionization and attachment processes. Applying those assumptions, the Boltzmann equation minimizes to a convection-diffusion continuity-equation. The last equation has no term of local source in energy space. It then discretized by the exponential schema to determine the EEDF by using a standard matrix inversion technique. The physical and mathematical techniques that used in BOLSIG+ are described in the Ref [13], and a brief description of the whole inputs and outputs are found in Ref [14].

Results and Discussion

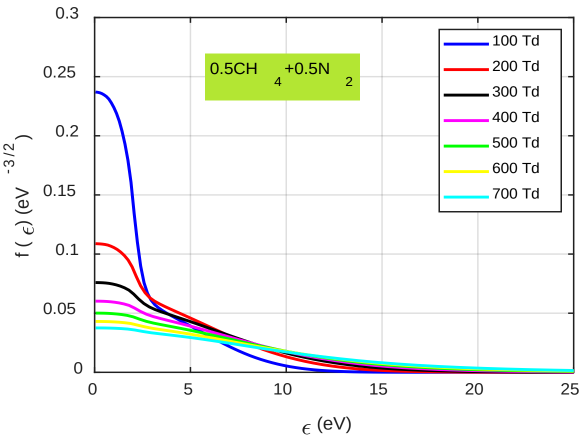

Figure 1. EEDF against the electron mean energy for different values for the $0.5CH_4 + 0.5N_2$ mixture

Fig. 1 represents the relationship between the EEDF and the electron mean energy for the mixture $0.5CH_4 + 0.5N_2$.It is noted that the EEDF decrease significantly when increasing the electron mean energy (0-4) eV, while the distribution function decreases slowly and gradually when the mean energy is greater than 4eV.The issue of changing the reduced electric field 100-700Td is observed on the EEDF, as it gets readable that the increases the reduced electric field, the EEDF decreases. This behavior applies when the value the electron mean energy is less than 10eV,while a behavioral reversal occurs when the value of the electron mean energy is greater than 10 eV.

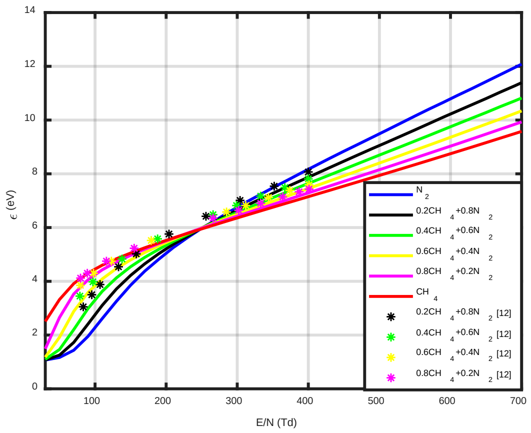

Figure 2. Electron mean energyϵ of mixtures with different concentrations of methane and nitrogen versus E/N

Fig. 2 shows the relationship between the electron mean energy of methane and nitrogen mixtures against the reduced electric field. The latter is defined as the ratio of electric field E to number density of the gas particles N. The curves increase exponentially at a value less than 250 Td; after this value the electron mean energy curves increase linearly toward the higher values of the reduced electric field. The results of the program were compared with the results of previous theoretical research and were in relatively good agreement [12].

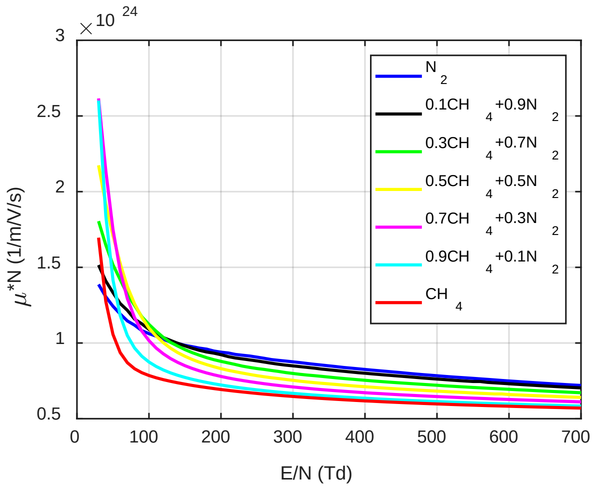

Figure 3. Mobilityμmultiplied by N of mixtures with individual concentrations of methane and nitrogen versus E/N

Fig. 3 shows the relationship between the mobility multiplied by the $N$for methane, nitrogen and the mixture of them versus the reduced electric field. The mobility curves of two gases and their mixtures gradually decrease with increasing values of the reduced electric field. Obviously, the mobility of nitrogen is higher than that for methane. They have similar mobility at value less than 40Td of E/N. For the $0.1CH_4$+$0.9N_2$ mixture, the curve has higher mobility than nitrogen at value of E/N less than 140Td, but after this value the curve of this mixture lay below the curve of nitrogen. Similar behavior for the other mixtures, however, the $0.9CH_4$+$0.1N_2$ mixture, the curve shifts down nearly the methane curve.

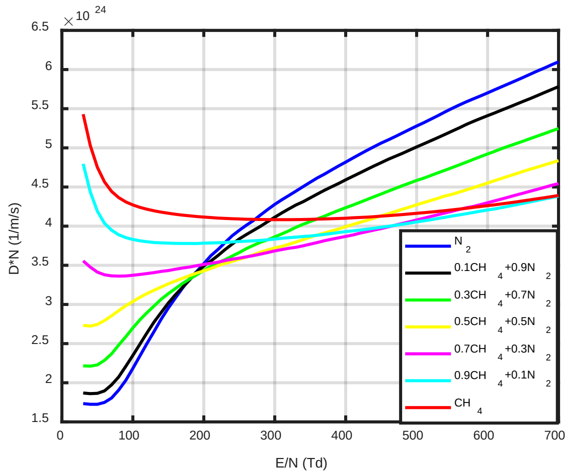

Figure 4. Electron diffusion coefficient D multiplied by N for pure nitrogen, methane and their mixtures of individual concentrations versus E/N.

Fig. 4 shows the relationship between the diffusion coefficient of electrons for methane and nitrogen mixtures against the reduced electric field. The graphs indicate different behavior of both gases. The electron diffusion coefficient for nitrogen increases exponentially, while it decreased exponentially for methane. The 0.9CH4+0.1N2 mixture reduces the diffusion coefficients compared to the methane for the used range of E/N. The others mixtures have common properties of the two gases depending on the ratio of the mixtures. The diffusion coefficients are lower than that of methane at lower E/N but higher at higher E/N relying on the ratio of the gases.

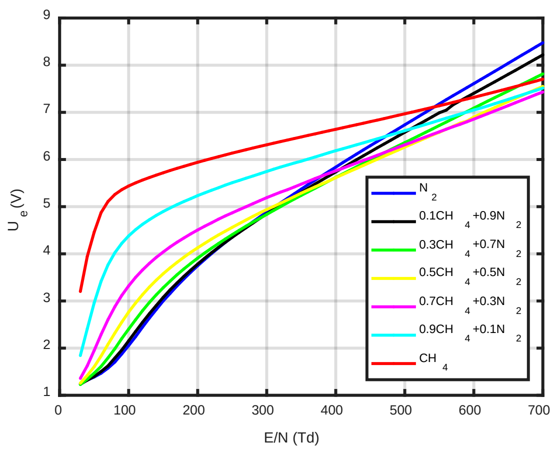

Figure 5. Characteristic energyU_e of mixtures with individual concentrations of methane and nitrogen versus E/N.

Fig. 5 shows the relationship between the characteristic energy of the methane and nitrogen mixtures against the reduced electric field. The characteristic energy is calculated by divide the pure electron diffusion D over the pure mobility μcoefficients.From the graph, it is clear that the more nitrogen concentrations mixture increase, the curves shift upwards.

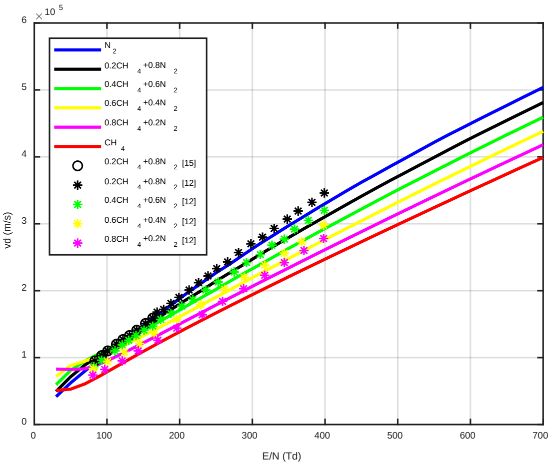

Figure 6. Electron drift velocityv_d for the mixtures with even concentrations of methane and nitrogen versus E/N.

Fig. 6 shows the relationship between the electron drift velocityv_d of methane and nitrogen mixtures against the E/N. Using the data of mobility calculated in the program, the drift velocity may be calculated through the formula $v_d = \mu/E$. The curves of the drift velocity increase linearly for all the concentrations shown in the figure at higher E/N. Notice that the special curves of the mixture concentrations are between the curve of methane and pure nitrogen. At lower E/N, the $0.8CH_4$+$0.2N_2$ mixture has higher velocity than methane and increased in similar manner. However, the calculations of the program look like the previous theoretical research in their behavior, but there are lower the curves of the references at low E/N and higher than the compared data as the E/N increased. The reason for this may be due to different data of cross sections used.

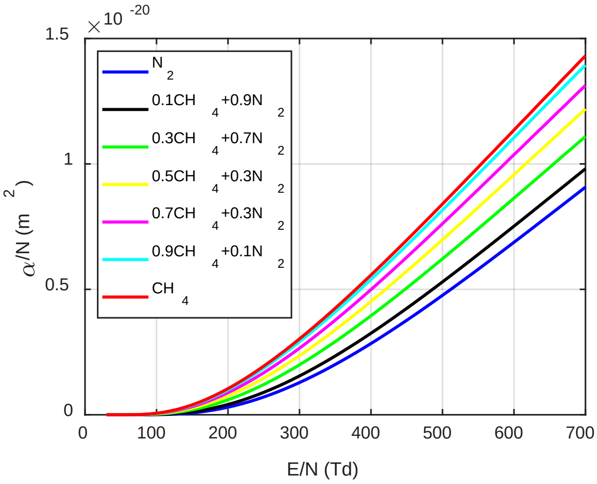

Figure 7. Townsend ionization coefficient (α/N) for mixtures of individual concentrations of methane and nitrogen versus E/N.

Fig. 7 shows the relationship between the Townsend ionization coefficient for methane and nitrogen mixtures against the reduced electric field. The figure shows that the increasing is an exponential relationship between the Townsend coefficient and the reducing electric field. It can be understood that the curves exhibit the same behavior all in the case of an increase in the methane concentration, or a reduction in the nitrogen concentration in the mixture, where the curves rise to the top and behave in as a pure methane behavior.

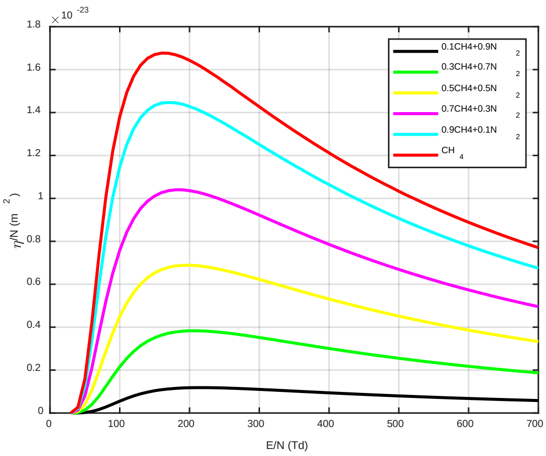

Figure 8. Townsend ionization coefficient (η/N) for mixtures with individual concentrations of methane and nitrogen versusE/N

Fig. 8 shows the relationship between the Townsend ionization factor for methane and nitrogen mixtures against the reduced electric field. From the graph of the curves, it can be seen that the Townsend coefficient of ionization shifts upward when the concentration of methane in the mixture increases, until these curves reach their highest peaks at less than 200Td. After this value, the curves gradually decrease toward the higher values of the reduced electric field.

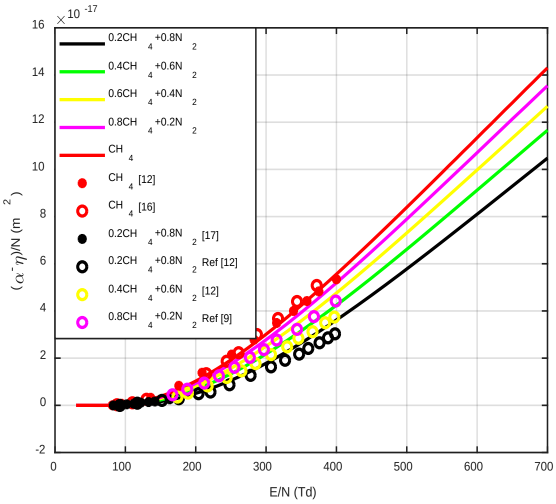

Figure 9. Effective ionization coefficient $(\alpha-\eta)/N$ for mixtures with even concentrations of methane and nitrogen versusE/N

Fig. 9 shows the relationship between the effective ionization factor of methane and nitrogen mixtures against the reduced electric field. The graph indicates that the effective ionization coefficient increases exponentially as the values of the E/N increase. These calculated results in the program were compared with the researchers' theoretical results. The different among them may be due to using different cross sections data.

Conclusions

We utilize the BOLSIG+ freeware to evaluate the electron transport coefficients and swarm parameters for pure methane, nitrogen and their mixtures in the range of reduced electric field varied from 30 to 700 Td. Generally, the program is of high credibility as indicated by the researchers in the field of low temperature plasmas. Therefore, the results of the calculations in this paper are accurate. Nevertheless, there is certainly mismatch between the results of the program and other mentioned researchers, due to different assumptions involved in the manner of solving the Boltzmann equation. In addition, using different cross section data causes different results. For a given value of E/N lower than 250Td, increasing nitrogen concentration in the gas mixtures leads to decrease electron mean energy, while it increased after this value of E/N. The characteristic energy decreases as the nitrogen content increased at low E/N, but it holds a reverse behaviour at high E/N. The drift velocity curves that depends on pure electron diffusion and the pure mobility coefficients show linear behavior with increased value of the E/N for all the methane-nitrogen mixtures. For a certain E/N, the effective ionization parameter decreases as the nitrogen concentration increases. The effective ionization parameter is more detectable at higher E/N value.

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BOLSIG+ can be downloaded from www.bolsig.laplace.univ-tlse.fr

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