



Study the Effect of Mixture (CHF_3 -He) Gasses on the Electronic Transmission Parameters During the Electrical Discharge Utilizing Programmatic Computer Analysis

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Abstract: This research examines The Electron Energy Distribution Function (EEDF) of electrons in plasma discharge for (CHF_3 -He) gas combinations. The Fortran programming language was used to solve the Boltzmann equation. A two-term approximation was used to solve the Boltzmann transport equation for both pure gases and mixtures. Using this method of solution, the electron energy distribution function was computed, and electric transport parameters were evaluated with range of E/N varying from (10–600) Td. The electron energy distribution function of the CHF_3 -He gas mixture is nearly Maxwellian at E/N values (10–20) Td, the distribution function is non-Maxwellian when E/N is raising. Also, the energy values of the mixtures largely depend on the transport energy between electron and molecule through collisions. In compared to mixtures, Helium gas has a high energy characteristic. At higher helium ratios, the mean electron energy to mixture is increasing. The mean electron energy in a gas mixture (35% CHF_3 + 65% He) and the behavior variation in electron mobility at this ratio both have larger values than other ratios.

Keywords: Electrical discharge; Plasma parameters; Mobility of electron; Boltzmann equation; Ionization coefficient

1 Introduction

Electric discharge has prominent applications in plasma generation and separation of electrical circuits. In addition to conducting experiments on gas discharge, numerical simulations are an essential study methodology to understand the discharge process. Some of the relevant physical parameters that should be known include the electron collision ionization coefficient, recombination coefficient, adhesion coefficient, mobility coefficient, and diffusion coefficient. The first Townsend's ionization coefficient and its symbolized by the symbol (α -coefficient) is the most important one for numerical gas discharge simulations [1].

The processes that result in the gas systems which gives rise to an electrical breakdown is termed as an electrical ionization system along with secondary electron emission. In the first phase of the ionization process where the incoming electron possess energy greater than the minimum required to ionize an electron in a molecule of gas, that particular electron will leave the molecule by forming a positive molecular ion. On the other hand, the second phase occurs when the energy emitted due to the recombination of positive ion along with the negative cathode drawn electron is greater than the work function energy of the electron within the conduction band of the cathode, which is the energy barrier between the vacuum and electron band [2].

Direct measurement of the Electron Energy Distribution Function (EEDF) is very impossible, yet it is crucial for predicting electron swarm characteristics. The EEDF is calculated from a set of electron gas collision cross-sections using the Boltzmann equation (two-term or multi-term solutions) or Monte Carlo simulation. Inelastic collisions can be solved using the two-term method when the electron collision frequency is different from the collision frequency for elastic collisions [3].

To start with, processes which electrons take part in are processes where their energy distribution function

determines their behavior. There is a considerable amount of elastic and inelastic collisions of electrons with normal and excited atoms, as well as molecules of the background gas and other regions varying through the electron transport process which forms the EEDF within certain limits, along with atoms and molecules of the background gas. Because in most cases the EEDF at high energy is non equilibrium, the finding of EEDF is considered as one of the main problems in determining the gas discharge features [4].

Trifluoroethane gas is produced when three of the four hydrogen atoms in methane are swapped out for halogen atoms, forming a haloform. It moves under its own vapor pressure as a liquefied gas (635 psig at 70° F). Trifluoroethane does not damage the ozone layer, despite being a greenhouse gas. One kind of pure hydro-fluorocarbon gas extinguishing agent that can be used in place of halon and chlorofluorocarbons is trifluoroethane (CHF₃). Its low boiling point, low toxicity, and insulating qualities are well-known, as is its capacity to extinguish electrical, flammable liquid, flammable gas, and solid surface fires. Prior to its introduction, little is known about the thermal properties and by products of this extinguishing chemical due to the necessity of replacing Halon. The microelectronics sector uses CHF₃ gas to etch silicon compounds. It is therefore very interesting to create reaction processes for gas mixtures, including CHF₃, for use in computer simulations of plasma processing reactors. Reviews and analysis of basic facts that are currently available [5, 6]. Thus, up to electron energies of roughly 2 eV, the momentum transfer cross section of electrons in helium gas is almost constant [7]. Since the electrons and the gas are in thermal equilibrium at low (E/N), $T_e = T_g$, the momentum transfer cross section of electrons for the entire inelastic collision system drops as energy increases. As (E/N) grows, the average electron temperature climbs well above this threshold. In the basic scenario, when only the elastic cross section is constant, T_e expands linearly with higher E/N values than T_g ; though, the elastic collision cross-section varies with the electron energy.

Using the Monte Carlo approach and taking into account inelastic collisions, the kinetic characteristics of electron drift in three inert gases (He, Ar, and Xe) with trace impurities equal to 1% of mercury vapor at an Electric Field Intensity (E/N) = 1–2000 Td were determined [8].

In order to ascertain the properties of their electrical transmission under fixed conditions, two types of gases (CHF₃/He) with three different weight ratios were employed. Additionally, the Boltzmann equation for the first and second approximations for different electric field strengths from (10–600 Td) can be solved using a computer program created in the Fortran language.

This study will use plasma parameters like average electron energy, ionization coefficient, correlation coefficient, electron mobility, and drift speed to determine the distribution functions and electric discharge behavior when using mixtures with varying concentrations.

2 Theoretical Part

2.1 Boltzmann Equation for Collisions

A Finite Difference iterative approach is used in the Fortran simulation to solve the two-term Boltzmann equation. In order to minimize numerical error, the convergence is strictly set when the relative change in the mean electron energy is smaller than 10^{-6} . The reliability of the model was validated by comparing its calculated transport parameters for pure gases with published experimental data, which showed strong agreement.

Here is a brief explanation of the computation technique. (M) stands for Molecular Mass, (E) for applied electric field strength, and (N) for gas density in the equations below. Townsend's initial attachment and ionization coefficients. The electron's mass and charge are denoted by (m) and (e). The electron's kinetic energy is denoted by ϵ . vibrational excitation, ionization, attachment, and electronic excitation are denoted by the subscripts i , a , v and ex , respectively. The electron collision cross-section is denoted by (Q) is the electron collision cross-section, and the subscripts represent the threshold energies of the inelastic collisions. The effective cross-section is denoted by Q_{em} [9, 10].

So as to determine the Electron Distribution Function, the fundamental equation is the Boltzmann equation. requires a steady electric field and a uniformly dispersed gas. According to Fridman [11], this equation uses the two terms estimate of the Boltzmann Equation for electrons in the collision state.

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial r} - \frac{e\vec{E}}{m} \frac{\partial f}{\partial v} = \left(\frac{df}{dt} \right)_c \quad (1)$$

where, $f: f(\vec{r}, \vec{v}, t)$ is the rate at which of $f(\vec{r}, \vec{v}, t)$ a changes due to $\left(\frac{df}{dt} \right)_c$ collision; hence, collisions are considered.

While the total derivative depicts all particles moving across the phase space, the partial derivative $\frac{\partial f}{\partial t}$ represents the change in the number of electrons at a particular location in the phase space. Where the total derivative is $\frac{df}{dt}$ represents all particles traveling in the phase space.

Now, one considers the situation of a spatially uniform gas that is solely a function of velocity $\nabla_r f = 0$ where Eq. (2) becomes:

$$\frac{\partial f}{\partial t} - \frac{e\vec{E}}{m} \nabla_v f = \left(\frac{df}{dt} \right)_c \quad (2)$$

Now consider only collisions between electron-atoms that are neutral. Calculating the contribution of each kind of collision to the shift in the distribution function is quite simple. Collisions can be classified as either inelastic or elastic:

$$\left(\frac{df}{dt} \right)_c = \left(\frac{df}{dt} \right)_{\text{elastic}} + \left(\frac{df}{dt} \right)_{\text{inelastic}} \quad (3)$$

The first part of Eq. (6) shows the function change caused by elastic collisions, while the second part shows the function change caused by inelastic collisions. The class of inelastic collisions also includes the creation of new electrons due to ionization, but not the excitation of atoms or molecules. Two equations remain after correction (approximation in two terms):

$$\frac{\partial f_0}{\partial t} - \frac{e\vec{E}}{m} \frac{1}{3v^2} \frac{\partial}{\partial v} (v^2 f_1) = \left(\frac{df_0}{dt} \right) \quad (4)$$

$$\frac{\partial f_1}{\partial t} - \frac{e\vec{E}}{m} \frac{\partial f_0}{\partial v} = \left(\frac{df_1}{dt} \right)_c \quad (5)$$

where, f_0 is the essential function (first approximation) and f_1 is the sconded approximation. The decrease in asymmetry in the distribution function is mostly caused by momentum-transfer collisions when the electron collision frequency for momentum-transfer is significantly higher than the electron collision frequency for excitation. According to Cao et al. [12], the following is the function change in the state of elastic collisions:

$$\left(\frac{df_1}{dt} \right)_c = -v_e(v) f_1(\vec{v}) \quad (6)$$

where, v_e is the electron momentum-transfer collision frequency where $v_e(v) = NQ_m(v)v$,

$$\left(\frac{df_1}{dt} \right)_c = -NQ_m(v) v f_1(\vec{v}) \quad (7)$$

Q_m is a cross section of a momentum transfer, N is the number density and v is the electron velocity. Whenever it is assumed that all quantities are time-independent: In elastic collisions, the change of function is provided by:

$$\frac{\partial f_0}{\partial t} - \frac{2e}{mv} \frac{\partial}{\partial \varepsilon} \left[\frac{\vec{E}^2 \varepsilon}{3NQ_m} \frac{\partial f_0}{\partial \varepsilon} + \frac{2m}{M} NQ_m \varepsilon^2 f_0 + \frac{2mK_B T}{Me} NQ_m \varepsilon^2 \frac{\partial f_0}{\partial \varepsilon} \right] = \left(\frac{df_0}{dt} \right)_c \quad (8)$$

where, K_B is Boltzmann constant, m is electron mass and M is Molecular mass.

The distribution function's evolution in a system with elastic collisions, thermal effects, and outside forces is described by this equation.

The equation you have provided relates the change in the distribution function $f_l(v)$ at the external electric field applied (E), the velocity v and the original distribution function f_0 . It appears to be a part of a kinetic theory framework, specifically dealing with the evolution of the distribution function of electron with influence the electric field is given by the relation:

$$f_1(\vec{v}) = \frac{e\vec{E}}{mvNQ_m(v)} \frac{\partial f_0}{\partial v} \quad (9)$$

2.2 Cross-Section of a Collisions

Tetrafluoromethane (CHF_3) values are dependent on the Cross Section sets both types elastic and that were published by Raju [13] and Kushner and Zhang [14], respectively. There are 16 collision processes in this collection, including three Vibration Excitations (Qv1, Qex, and Qa) with threshold energies and one momentum transfer cross section (Q_m).

2.3 Transport Coefficients and Plasma Electric Discharge Parameters

Transport phenomena are the processes associated with the movement of mass, momentum, energy, and charges in plasma. In this work, the transport coefficients were calculated.

In contrast to carriers in free space, carriers in semiconductors get a fixed velocity regardless of how long the electric field is acting since they are not "infinitely" driven by it due to scattering. The carrier mobility is found at a certain electric field drift velocity. When an electron collides, it accelerates along the line of force of the electric field in the area between collisions.

The following equation states that the electron energy distribution function can become a Maxwellian distribution when the normalization condition is happened [13]:

$$f(\varepsilon) = \frac{1}{N_S} \frac{4\pi}{m} \sqrt{\frac{2}{m}} f_0(\varepsilon) \quad (10)$$

Additionally, the following mathematical relationship can be used to determine the average electron energy:

$$\langle \varepsilon \rangle = \int_0^\infty \varepsilon^{\frac{3}{2}} f(\varepsilon) d\varepsilon \quad (11)$$

A collision causes the motion to change randomly and rapidly, which accelerates the electron once more. In a weakly ionized gas, neutral molecules are more possible to collide than charged particles. The methodical movement toward the external force in the face of random motion is known as drift [12].

The mobility depends on the strength of the electric field, and the drift velocity (v_d) is a nonlinear function of the electric field. The drift velocity is proportional with (E/N) , where an electron loses all of its energy equivalent to the gain from the electric field in a single elastic contact. There is a correlation between drift velocity and the electron energy distribution function [12]:

$$v_d = -\frac{E}{3} \left(\frac{2e}{m} \right)^{\frac{1}{2}} \int_0^\infty \frac{u}{NQ_m(u)} \frac{df_0}{du} du \quad (12)$$

The mobility is the proportional coefficient between the strength of an electric field and the Drift Velocity of a charged particle. The Mobility (μ_e) of the electrons is given by the relation:

$$\mu_e = \frac{e}{mv_m} = \frac{v_d}{E} \quad (13)$$

where, v_m is the frequency of collisions between electrons that transfer momentum. Electron mobility dropped with increasing E/N . Collisions between electrons and neutral molecules resulted in energy loss. With EEDF, we can use the relationship between drift velocity and mobility to obtain the electron mobility equation [1]:

$$\mu_e = -\frac{1}{3} \left(\frac{2e}{m} \right)^{\frac{1}{2}} \int_0^\infty \frac{u}{\sum \delta_s Q_m(u)} \frac{df_0}{du} du \quad (14)$$

where, δ_s represents fractional concentration of the s species $\delta_s = \frac{N_s^i}{N_s}$ and N_s^j is the number of molecules of species s in the excited state j , free diffusion is the independent diffusion of charges with opposing signs when the density of charged particles is relatively low.

The ambipolar diffusion coefficient in a weakly ionized gas discharge is simplified by noting that the relationship between the electron energy distribution function and diffusion coefficient and is usually specified by Brush [15].

$$D_T = \frac{1}{3} \left(\frac{2}{m} \right)^{1/2} \int \frac{u^{1/2}}{NQ_m(u)} f(u) du \frac{1}{n} \quad (15)$$

Electron attachment is the process in which an electron collides with a neutral atom to form a negative ion. Both dissociative and non-dissociative electron attachment reactions depend strongly on electron energy. The following relation describes the rate of attachment:

$$R_a = \left(\frac{2}{m}\right)^{1/2} \int_{\varepsilon} N Q_a(\varepsilon) f(\varepsilon) d\varepsilon \quad (16)$$

The energy distribution function of electrons is normalized to unity where and the attachment cross section. In plasma kinetics, the rate of electron attachment directly explains the loss of electrons and the rise in the density of negative ions. The relationship: provides the electron attachment coefficient is:

$$\frac{\eta}{N} = \frac{1}{v_d} \left(\frac{2}{m}\right)^{1/2} \sum_k \int_{ik} \frac{N_K}{N} Q_{ak}(u) u f_0(u) du \quad (17)$$

The drift velocity is given by [16]:

$$v_d = \left(\frac{1}{ne}\right) \int_0^{\infty} \sigma v f(\varepsilon) d\varepsilon \quad (18)$$

3 Results and Discussion

The Townsend region, which is confined between (10–500) Td, was used to study the electron velocity distribution function. As shown in Figure 1, the results demonstrated that the values $f(v)$ have a Maxwellian distribution to satisfy the distribution condition at that point, and that the distribution becomes non-Maxwellian as the intensity of the applied electric field increases. By contrasting the computed mean electron energy in pure He gas with the findings reported by Hagelaar and Pitchford [16] and Yuan et al. [17], The sequence of operations to reach the results can be illustrated by the simple flow chart below in Figure 1.

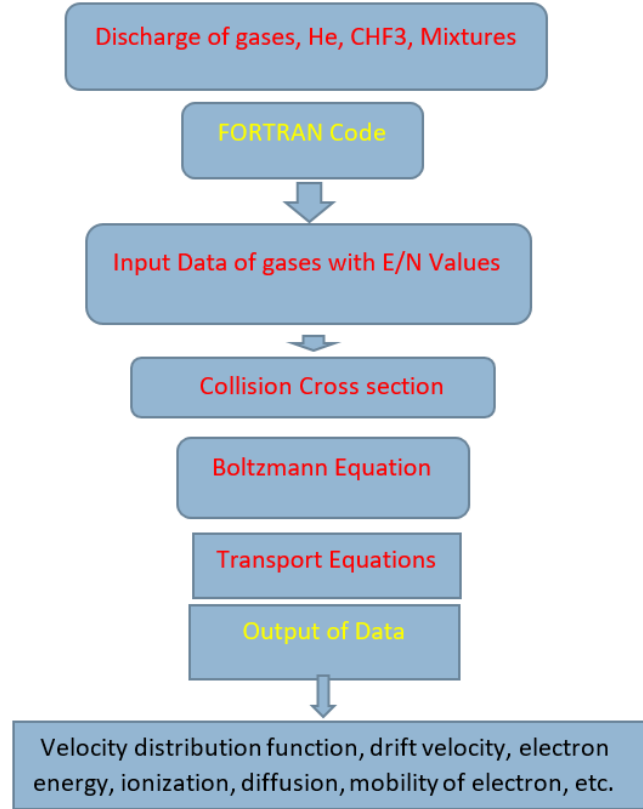


Figure 1. Flowchart of the computational procedure for evaluating electron transport parameters in pure gases and CHF₃/He mixtures

The range of 10–500 Td, Figure 2 illustrates the validation of the numerical model. Excellent agreement is shown by the results. This robust correlation validates the dependability of the He cross-section set and the Fortran code utilized in this investigation, supporting its later use with the CHF₃/He combinations.

The relationship between an electron's energy and velocity distribution function is depicted in Figure 3. For the E/N values (10,20) Td, the distribution function seems to be roughly Maxwellian (reduced power losses); this is consistent with a state of thermal equilibrium (isotropic distribution). Inelastic collisions alter the Electron Energy Distribution for (E/N) > 20 Td, and gas atoms become excited, limiting the electrons' mean energy and producing a non-Maxwellian distribution [18–20]. This study focused on the weakly ionized Townsend region, which exhibits a difference in power and current generation compared to high-discharge regions such as arc discharges. It suffers from limitations due to the complexity of its input parameters, making it an inaccurate study [21].

The mixture (35% CHF₃ /65% He) gas mixtures in Figure 3 have a high mean electron energy, meaning that the electrons' energy reaches roughly 2.5 electron volts, indicating that there is a small energy loss during the collision. Due to the presence of energy convergence in other mixtures, Figure 4 shows a higher degree of freedom for the electrons in mobility with an energy gain for the electrons in inelastic collision with atoms [22, 23].

Figure 5 shows that the ionization coefficient increases from E/N up to 200 Td, after which it noticeably decreases till 600 Td. This suggests that collisions or ion arrival at the cathode electrode result in energy losses, which lowers the ionization coefficient. A mixture of (85% CHF₃/15% He) had the optimal ratio [24, 25].

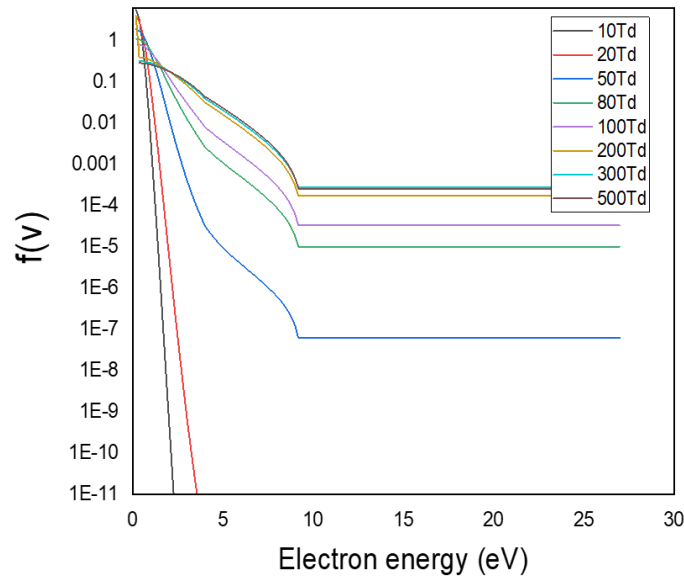


Figure 2. Electron energy distribution functions (EEDFs) of CHF₃/He mixtures at different reduced electric fields (E/N)

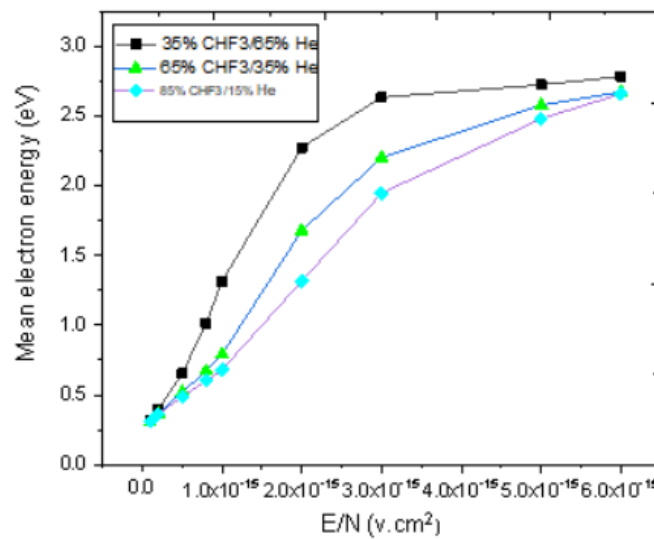


Figure 3. Mean electron energy as a function of reduced electric field (E/N) for different CHF₃/He mixture ratios

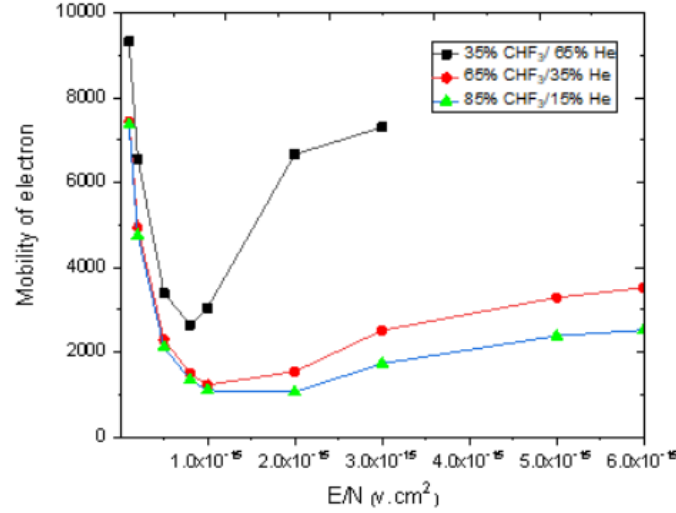


Figure 4. Electron mobility as a function of reduced electric field (E/N) for various CHF_3/He gas mixtures

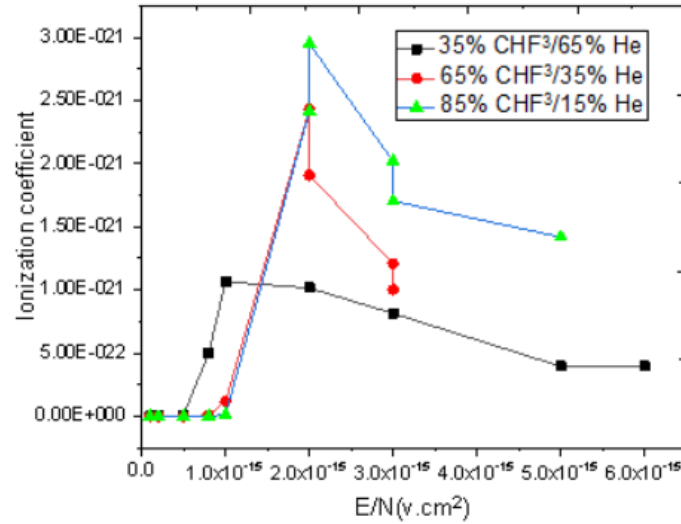


Figure 5. Ionization coefficient versus reduced electric field (E/N) for different CHF_3/He mixture compositions

It is obvious from the results in Figure 6 that electrons have a diffusion coefficient. Diffusion was most prevalent in gas mixtures, indicating the strength of the electric field and the absence of energy losses from electron-atom collisions [26, 27].

The relationship between the drift velocity and the E/N ratio can be explained using kinetic theory, as shown in Figure 7. These results are consistent with Dandapat and Rays' results [28]. An electron swarm wanders at a velocity due to the thermal motion of the electrons below the effect of an Electric Field E .

The relative magnitudes of the elastic power fraction, vibrational fraction, and ionization fraction are plotted against the reduced electric field (E/N) in this log-log plot, which ranges from $\approx 10^{-6}$ to 10^{-16} V cm^2 as shown in Figure 8. The vibrational processes are the predominant energy transfer route in this system across the whole E/N range, as indicated by the red line, which represents the vibrational fraction, remaining dominating and constant at a value of 1. The ionization fraction, or black line, begins very low and rises sharply at about $E/N \approx 10^{-18}$ V cm^2 , indicating the beginning of heavy ionization. However, it saturates at a low level ($\approx 10^{-2}$), indicating that it is a small channel in comparison to vibrational excitation. Likewise, the elastic power fraction, represented by the blue line, continuously remains low. However, compared to vibrational excitation, it saturates at a low level ($\approx 10^{-2}$), indicating that it is a minor channel. Elastic collisions are negligible energy loss mechanisms in this domain, as shown by the blue line, the elastic power fraction, which likewise continually maintains a low value, likewise falling between 10^{-3} and 10^{-2} for high E/N [29, 30].

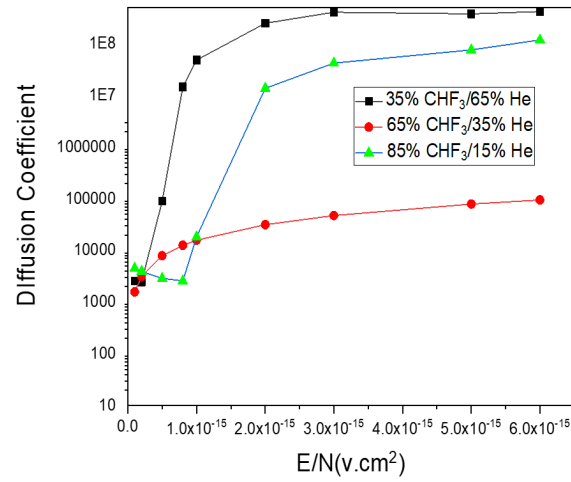


Figure 6. Diffusion coefficient as a function of reduced electric field (E/N) for CHF_3/He mixtures

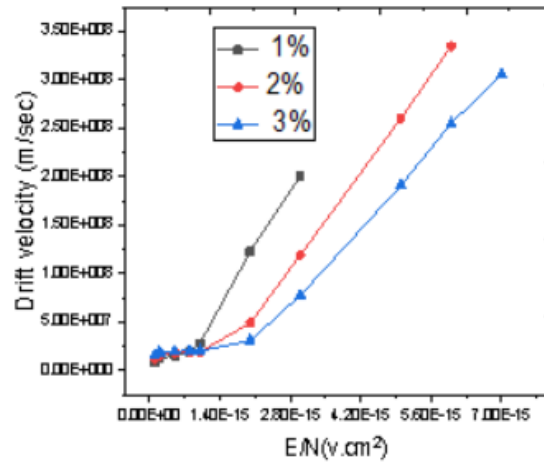


Figure 7. Electron drift velocity versus reduced electric field (E/N) for various CHF_3/He mixture ratios

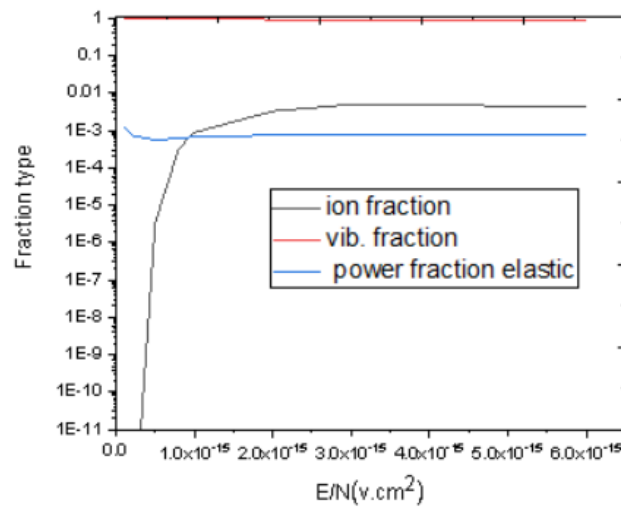


Figure 8. Fractional power loss contributions as a function of reduced electric field (E/N)

4 Conclusion

This work provides new insights into how the behaviour of electron transport and plasma characteristics in CHF₃-He gas mixtures are influenced by varying electric field strengths. As the E/N grows, electrons change from having a Maxwellian distribution at low E/N (10–20 Td) to a non-Maxwellian form, indicating the growing importance of inelastic collisions and energy loss mechanisms. The 35% CHF₃ + 65% He mixture shows enhanced mean electron energy and mobility, which is suitable for stable, high-energy plasma discharges since helium effectively facilitates energy transfer. 85% CHF₃ + 15% He shows higher ionization efficiency. However, he suggests that it might be used in processes that require more ionization control, such as plasma-assisted etching. These findings expand on our knowledge of how halocarbon-helium combinations affect plasma transport properties and offer practical suggestions for optimizing gas ratios in commercial plasma technologies and computational discharge modeling. The work also demonstrates the accuracy of the Fortran-based Boltzmann solver in predicting plasma properties in mixed-gas environments.

Data Availability

The data used to support the findings of this study are available from the corresponding author upon request.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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