Theoretical Calculation of the Electron Transport Parameters and Energy Distribution Function for CF3I with noble gases mixtures using Monte Carlo simulation program

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Abstract. In this paper, The Monte Carlo simulation program has been used to calculation the electron energy distribution function (EEDF) and electric transport parameters for the gas mixtures of The trifluoroiodomethane (CF3I) ‘environment friendly’ with a noble gases (Argon, Helium, Kryptos, Neon and Xenon).

The electron transport parameters are assessed in the range of E/N (E is the electric field and N is the gas number density of background gas molecules) between 100 to 2000 Td (1 Townsend =10^-17 V cm2) at room temperature. These parameters, namely are electron mean energy (ε), the density -normalized longitudinal diffusion coefficient (NDL) and the density –normalized mobility (μN).

In contrast, the impact of CF3I in the noble gases mixture is strongly apparent in the values for the electron mean energy, the density –normalized longitudinal diffusion coefficient and the density –normalized mobility. Note in the results of the calculation agreed well with the experimental results.

1. Introduction

The electron transport parameters have been studied for a wide range of applied electric field. These parameters, such as, the drift velocity, mobility, diffusion coefficient, ionization coefficient, and electron mean energy are knowledge in collision cross section and EEDF personification the backbone of the electron swarm behavior of gas in discharge of plasma [1].

The numerical solution of the Boltzmann EQUATION yields the electron energy distribution with the electric field E and gas number density N as parameters.

trifluoroiodomethane (CF3I) has been found to be a potential high voltage insulator[2,3]. Generally, CF3I is colorless and nonflammable [4,5]. From an environmental point of view, CF3I presents a weak global warming potential (GWP) of 1–5 against approximately 23900 for SF6[6,7].

CF3I is considered as a low environmental impact gas and is attracting widespread attention for comprehensive study. However, CF3I has a high boiling point -22.5 C0, as reported in Ref. [8,9].

The electron transport in a gas under the effect of an electric field E can be simulated with the help of a Monte Carlo method [10-15].

In this work the Monte Carlo simulation technique for ion transport that accounts for limited gas temperature is used to calculate electron transport parameters of CF3I with noble gas mixture at temperature T=300 K. transport parameters are determined as a function of E/N for various rates of increase of the electric field [16].

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In this paper is calculation the electron energy distribution function and electron transport parameters for trifluoroiodomethane mixtures with a noble gases (Argon, Helium, kryptos, Neon and Xenon) by using Monte Carlo simulation program.

2. Theory

The Boltzmann equation describes the time evolution of the electron energy distribution function $f(r, v, t)$.

The Boltzmann equation for electrons in an ionized gas is [17]:

$$\frac{\partial f}{\partial t} + V \cdot \nabla f - \alpha \cdot \nabla f = \beta(f)$$

Where $\alpha = -eE/m$ represents the acceleration of the electrons due to the external electric field $E$, and $\beta$ is the collision operator.

The Boltzmann equation maybe written as [18,19]:

$$\left( \frac{\partial}{\partial t} + v \cdot \nabla_r + \frac{eE}{m} \cdot \nabla_V \right) f(r, v, t) = \left( \frac{\delta}{\partial t} \right)$$

where $f(r, v, t)$ is the electrons distribution at time t and spatial location r, $v$ is the velocity of charge particles and $\nabla_V$ is the gradient in V-space.

The electron mean energy is, [22,23]:

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

Values of $f_0$ are calculated from Boltzmann’s equation using all collision cross-sections.

The relation between drift velocity $w$ and distribution function of electron energy is given by [24,25]:

$$w = -\frac{1}{3} \left( \frac{2}{m} \right)^{1/2} \frac{eE}{N} \int_0^\infty \frac{e}{q_m(\varepsilon)} d\varepsilon$$

Where $\varepsilon$ is the electron energy in (eV), $m$ is the electron mass, $e$ is the elementary charge and $q_m$ is the momentum transfer cross section (in cm2).

The mobility is defined as the proportionally coefficient between the drift velocity of a charged particle and electric field. The mobility of electrons is (in cm²/V)[26,27]:

$$\mu_e = \frac{e}{m_{pe} E}$$
Where $\nu_m$ represent the electron momentum-transfer collision frequency.

The density-normalized mobility ($\mu N$) is defined as:

$$
(\mu N) = -\frac{\partial}{\partial N} \int_0^\infty \frac{e^{\gamma/2}}{\frac{qT}{\partial N}} \frac{\partial f_0}{\partial N} d\varepsilon .
$$

And the density-normalized longitudinal diffusion coefficient is defined as:

$$
ND_L = \frac{V_1}{2N} \left[ B \int_0^\infty \frac{e^{\gamma/2}}{\frac{qT}{\partial N}} (f_1 \varepsilon^{-1/2}) d\varepsilon + \int_0^\infty \frac{e^{\gamma/2}}{qT} f_0 d\varepsilon \right] - (\bar{w}_0 A_2 - \bar{w}_1 A_1 - \bar{w}_2) .
$$

Where $V_1$ is the speed of electron, $q_T$ is the total cross section, $f_n$ and $n$ ($n = 0, 1, 2$) are respectively the electron energy distributions of various orders and their eigen values. $V_1$, $n$ ($n = 0, 1, 2$), and $A_n$ are given by [28-30]

$$
V_1 = \left( \frac{2e}{m} \right)^{1/2}.
$$

$$
\bar{w}_0 = V_1 N \int_0^\infty \varepsilon^{1/2} q_0 f_0 d\varepsilon .
$$

$$
\bar{w}_1 = -\frac{V_1}{3N} \int_0^\infty \varepsilon^{1/2} q_1 f_1 d\varepsilon + (\bar{w}_0 A_1 - \bar{w}_2) .
$$

$$
\bar{w}_{01} = V_1 N \int_0^\infty \varepsilon^{1/2} q_1 f_0 d\varepsilon .
$$

$$
A_n = \int_0^\infty f_n d\varepsilon .
$$

Where $q_i$ is the ionization cross section.

3. Result

To calculate the electron mean energy and the others transport parameters using the Monte Carlo simulation program, find out about the accreditation of the momentum transfer cross section on the electron energy is basis, We present the results of The electron mean energy, the density – normalized longitudinal diffusion coefficient and the density – normalized mobility as functions of $E/N$ for mixtures CF3I gas with noble gases (Ar, Kr, Xe, He and Ne) have been calculated in the $E/N$ range $100 < E/N < 2000$ Td are recorded in Table (1-6).

Tables (1-3) note the computed results for the electron mean energy, the density – normalized longitudinal diffusion coefficient and the density – normalized mobility as a function of $E/N$, respectively in pure CF3I and pure noble gases.

Tables (4) clarify the calculated results for the electron mean energy, in various ratios of CF3I mixtures with (Argon, Helium, kryptos, Neon and Xenon) gases.

Tables (5) clarify the computed results for the density – normalized longitudinal diffusion coefficient, in different ratios of CF3I mixtures with (Argon, Helium, kryptos, Neon and Xenon) gases.

Tables (6) explain the calculated results for the density – normalized mobility in various proportions of CF3I mixtures with (Argon, Helium, kryptos, Neon and Xenon) gases.
'Figure (1)' exhibit the behavior of the electrons energy dependence distribution function for different cases of the factor (E/N) and , figure (2) show the variety in the mean energy of electrons as a function of (E/N), which increases with increase of E/N and they appear clearly effect of adding noble gases (Argon, Helium, kryptos, Neon and Xenon) to the trifloroiodo methane (CF$_3$I) gas in increasing due to the change in the various types of collision processes.

Figure (3) show the density -normalized mobility for different ratios of mixtures CF$_3$I with noble gases, we notice that it decreases by increasing E/N.

The gas density normalized longitudinal diffusion coefficient $ND_L$, the product of the gas number density $N$ and the longitudinal diffusion coefficient $D_L$ for CF$_3$I mixtures with noble gases, is plotted in Figure (4) as a function of E/N.

in figure (5) for pure CF$_3$I. The results demonstrate a good agreement with the experimental values [31].

4. Conclusion

In this study, we have examined the behavior of electrons in uniform electric fields using a Monte Carlo simulation. Electron transport parameters were calculated as a function of reduced electric fields E/N.

   calculation the electron energy distribution function and the transport parameters for The trifloroiodo methane (CF$_3$I) ‘environment friendly’ with a noble gases (Argon, Helium, kryptos, Neon and Xenon) in the E/N range of 100 - 2000 Td.

In this work, the simulation results give values for electron mean energy, the density -normalized longitudinal diffusion coefficient (ND$_L$) the density -normalized mobility ($\mu N$) and electron energy distribution as functions of reduced electric field.

Table 1. The calculate electron Mean Energy(ε)( eV) in pure of CF3I and Noble gases (Ar, He, Kr, Ne and Xe).

| E/N(Td) | Xe | Ne | Kr | He | Ar | CF3I |
|--------|----|----|----|----|----|------|
| 100    | 4.486 | 12.87 | 5.607 | 12.82 | 6.666 | 2.938 |
| 200    | 4.642 | 13.93 | 5.827 | 14.87 | 6.978 | 3.215 |
| 300    | 4.819 | 15.25 | 6.078 | 18.12 | 7.275 | 3.52  |
| 400    | 5.025 | 16.85 | 6.361 | 23.64 | 7.61  | 3.846 |
| 500    | 5.272 | 18.81 | 6.998 | 32.44 | 8.012 | 4.191 |
| 600    | 5.578 | 21.23 | 7.106 | 44.96 | 8.507 | 4.557 |
| 700    | 5.969 | 24.3  | 7.614 | 61.71 | 9.134 | 4.946 |
| 800    | 6.484 | 27.88 | 8.262 | 83.97 | 9.955 | 5.366 |
| 900    | 7.18  | 32.45 | 9.106 | 113.9 | 11.006 | 5.829 |
| 1000   | 8.138 | 38.12 | 10.21 | 155.3 | 12.62 | 6.352 |
| 1200   | 9.472 | 45.21 | 11.67 | 215.1 | 14.94 | 6.963 |
| 1400   | 11.32 | 54.2  | 13.58 | 305.3 | 18.52 | 7.706 |
| 1600   | 13.83 | 65.89 | 16.03 | 449.9 | 24.18 | 8.901 |
| 1800   | 17.17 | 81.69 | 19.16 | 688.13 | 33  | 9.901 |
| 2000   | 21.52 | 104.1 | 23.08 | 1153 | 46.64 | 11.62 |
Table 2: The calculated density-normalized mobility ($\mu_N \times 10^{23} (\text{mVs})^{-1}$) for electron in pure of CF$_3$I and Noble gases (Ar, He, Kr, Ne and Xe).

| E/N(Td) | Xe  | Ne  | Kr  | He  | Ar  | CF$_3$I |
|---------|-----|-----|-----|-----|-----|---------|
| 100     | 5.444 | 24.16 | 7.356 | 2.83 | 8.195 | 6.84   |
| 200     | 5.431 | 22.91 | 7.196 | 3.14 | 7.847 | 6.365  |
| 300     | 5.441 | 21.66 | 7.052 | 3.638 | 7.651 | 5.986  |
| 400     | 5.476 | 20.43 | 6.924 | 4.39 | 7.494 | 5.675  |
| 500     | 5.537 | 19.23 | 6.814 | 5.267 | 7.359 | 5.41   |
| 600     | 5.631 | 18.07 | 6.719 | 6.019 | 7.247 | 5.178  |
| 700     | 5.764 | 16.92 | 6.642 | 6.514 | 7.167 | 4.969  |
| 800     | 5.945 | 15.89 | 6.58 | 6.772 | 7.138 | 4.779  |
| 900     | 6.175 | 14.87 | 6.535 | 6.83 | 7.169 | 4.604  |
| 1000    | 6.44 | 13.88 | 6.486 | 6.777 | 7.286 | 4.443  |
| 1200    | 6.727 | 12.93 | 6.413 | 6.674 | 7.496 | 4.295  |
| 1400    | 6.97 | 12.03 | 6.298 | 6.582 | 7.791 | 4.167  |
| 1600    | 7.123 | 11.2 | 6.115 | 6.559 | 8.152 | 4.066  |
| 1800    | 7.127 | 10.48 | 5.856 | 6.559 | 8.524 | 3.997  |
| 2000    | 6.988 | 9.914 | 5.528 | 6.896 | 8.82 | 3.95  |

Table 3: The calculated density-normalized longitudinal diffusion coefficient ($ND_T$) $\times 10^4$(m s$^{-1}$) for electron in pure of CF$_3$I and Noble gases (Ar, He, Kr, Ne and Xe).

| E/N(Td) | Xe  | Ne  | Kr  | He  | Ar  | CF$_3$I |
|---------|-----|-----|-----|-----|-----|---------|
| 100     | 4.034 | 25.15 | 7.346 | 24.27 | 6.761 | 1.985   |
| 200     | 3.963 | 25.66 | 7.026 | 32.94 | 6.594 | 1.993   |
| 300     | 3.881 | 26.27 | 6.65 | 52.11 | 6.457 | 2.009   |
| 400     | 3.791 | 27.03 | 6.237 | 94.28 | 6.332 | 2.031   |
| 500     | 3.7 | 27.97 | 5.849 | 164.6 | 6.23 | 2.06   |
| 600     | 3.613 | 29.17 | 5.517 | 255.1 | 6.167 | 2.093   |
| 700     | 3.553 | 30.62 | 5.275 | 359.3 | 6.17 | 2.133   |
| 800     | 3.576 | 32.47 | 5.147 | 479.4 | 6.289 | 2.179   |
| 900     | 3.726 | 34.74 | 5.159 | 622.5 | 6.597 | 2.233   |
| 1000    | 4.079 | 37.52 | 5.329 | 806.3 | 7.255 | 2.296   |
| 1200    | 4.702 | 40.9 | 5.671 | 1061 | 8.546 | 2.375   |
| 1400    | 5.641 | 45.11 | 6.194 | 1444 | 10.9 | 2.482   |
| 1600    | 6.911 | 50.6 | 6.881 | 2076 | 15.14 | 2.642   |
| 1800    | 8.499 | 58.42 | 7.705 | 3223 | 21.93 | 2.895   |
| 2000    | 10.36 | 70.56 | 8.64 | 5527 | 32.41 | 3.293   |

Table 4: The calculated electron Mean Energy($\varepsilon$( eV)) in various mixture of CF$_3$I with Noble gases (Ar, He, Kr, Ne and Xe).

| E/N(Td) | 20% $\varepsilon$( eV) | 40% $\varepsilon$( eV) |
|---------|------------------------|------------------------|
|         | Xe  | Ne  | Kr  | He  | Ar  | Xe  | Ne  | Kr  | He  | Ar  |
| 100     | 3.067 | 3.21 | 3.148 | 3.172 | 3.176 | 3.244 | 3.596 | 3.425 | 3.496 | 3.5 |
| 200     | 3.355 | 3.515 | 3.444 | 3.475 | 3.477 | 3.541 | 3.928 | 3.739 | 3.825 | 3.822 |
| 300     | 3.666 | 3.842 | 3.763 | 3.801 | 3.8 | 3.851 | 4.278 | 4.069 | 4.173 | 4.161 |
| 400     | 3.992 | 4.187 | 4.099 | 4.145 | 4.14 | 4.172 | 4.648 | 4.412 | 4.541 | 4.516 |
| 500     | 4.335 | 4.552 | 4.453 | 4.509 | 4.544 | 4.507 | 5.044 | 4.773 | 4.934 | 4.89 |
| 600     | 4.627 | 4.941 | 4.826 | 4.897 | 4.87 | 4.862 | 5.473 | 5.155 | 5.36 | 5.278 |
Table 5. The calculate density–normalized mobility (μN) (mVs)^{-1} for electron in various mixture of CF_4 with Noble gases (Ar, He, Kr, Ne and Xe).

| E/N(Td) | Xe | Ne | Kr | He | Ar | Xe | Ne | Kr | He | Ar |
|---------|----|----|----|----|----|----|----|----|----|----|
| 700     | 5.084 | 5.36 | 5.226 | 5.315 | 5.282 | 5.246 | 5.946 | 5.567 | 5.831 | 5.712 |
| 800     | 5.507 | 5.822 | 5.661 | 5.776 | 5.726 | 5.673 | 6.483 | 6.023 | 6.366 | 6.301 |
| 900     | 5.981 | 6.343 | 6.146 | 6.296 | 6.221 | 6.165 | 7.112 | 6.542 | 6.994 | 6.827 |
| 1000    | 6.53 | 6.949 | 6.706 | 6.902 | 6.79 | 6.754 | 7.876 | 7.156 | 7.763 | 7.445 |
| 1200    | 7.191 | 7.683 | 7.375 | 7.638 | 7.971 | 7.488 | 8.842 | 7.913 | 8.749 | 8.204 |
| 1400    | 8.018 | 8.61 | 8.211 | 8.571 | 8.322 | 8.439 | 10.11 | 8.884 | 10.07 | 9.181 |
| 1600    | 9.1 | 9.827 | 9.298 | 9.807 | 9.435 | 9.716 | 11.81 | 10.17 | 11.89 | 10.49 |
| 1800    | 10.56 | 11.48 | 10.76 | 11.5 | 10.95 | 11.47 | 14.13 | 11.91 | 14.42 | 12.47 |
| 2000    | 12.58 | 13.75 | 12.75 | 13.85 | 13.05 | 13.87 | 17.26 | 14.25 | 17.88 | 15.15 |

| E/N(Td) | Xe | Ne | Kr | He | Ar | Xe | Ne | Kr | He | Ar |
|---------|----|----|----|----|----|----|----|----|----|----|
| 60%     | μ (eV) | 4.179 | 3.812 | 3.973 | 3.962 | 3.889 | 5.26 | 4.411 | 4.825 | 4.712 |
| 80%     | μ (eV) | 4.544 | 4.137 | 4.333 | 4.303 | 4.147 | 5.706 | 4.73 | 5.258 | 5.068 |

| E/N(Td) | Xe | Ne | Kr | He | Ar | Xe | Ne | Kr | He | Ar |
|---------|----|----|----|----|----|----|----|----|----|----|
| 20% μN x 10^3 (m Vs)^{-1} | | | | | | | | | |
| 40% μN x 10^3 (m Vs)^{-1} | | | | | | | | | |
Table 6. The calculate density –normalized longitudinal diffusion coefficient (ND×) (m s)\(^{-1}\) for electron in various mixture of CF\(_3\)I with Noble gases (Ar, He, Kr,Ne and Xe).

| E/N(Td) | Xe | Ne | Kr | He | Ar |
|---------|----|----|----|----|----|
| 100     | 5.763 | 11.81 | 7.375 | 9.916 | 8.659 |
| 200     | 5.177 | 12.27 | 6.874 | 9.551 | 8.062 |
| 300     | 5.35 | 10.79 | 6.469 | 9.231 | 7.547 |
| 400     | 5.236 | 10.34 | 6.134 | 8.947 | 7.1 |
| 1000    | 5.154 | 9.925 | 5.85 | 8.693 | 6.757 |
| 2000    | 5.1 | 9.531 | 5.607 | 8.465 | 6.388 |
| 100     | 5.386 | 9.157 | 5.398 | 8.265 | 6.074 |
| 200     | 5.051 | 8.806 | 5.218 | 8.101 | 5.585 |
| 300     | 5.053 | 8.482 | 5.063 | 7.99 | 5.645 |
| 400     | 5.076 | 8.192 | 4.93 | 7.959 | 5.5 |
| 1000    | 5.124 | 7.937 | 4.822 | 8 | 5.418 |
| 1400    | 5.195 | 7.703 | 4.739 | 8.08 | 5.38 |
| 1600    | 5.277 | 7.462 | 4.681 | 8.141 | 5.4 |
| 1800    | 5.339 | 7.184 | 4.63 | 8.09 | 5.452 |
| 2000    | 5.34 | 6.851 | 4.564 | 7.9 | 5.477 |

| E/N(Td) | Xe | Ne | Kr | He | Ar |
|---------|----|----|----|----|----|
| 100     | 2.079 | 2.418 | 2.283 | 2.242 | 2.339 |
| 200     | 2.077 | 2.433 | 2.284 | 2.268 | 2.346 |
| 300     | 2.085 | 2.453 | 2.292 | 2.303 | 2.36 |
| 400     | 2.102 | 2.502 | 2.307 | 2.344 | 2.338 |
| 500     | 2.126 | 2.544 | 2.328 | 2.392 | 2.405 |
| 600     | 2.159 | 2.593 | 2.356 | 2.446 | 2.435 |
| 700     | 2.23 | 2.649 | 2.391 | 2.509 | 2.472 |
| 800     | 2.252 | 2.714 | 2.435 | 2.58 | 2.517 |
| 900     | 2.315 | 2.79 | 2.489 | 2.66 | 2.57 |
| 1000    | 2.396 | 2.88 | 2.559 | 2.767 | 2.639 |
| 1200    | 2.504 | 3.008 | 2.653 | 2.904 | 2.732 |
| 1400    | 2.659 | 3.188 | 2.791 | 3.106 | 2.872 |
| 1600    | 2.899 | 3.466 | 3.005 | 3.419 | 3.097 |
| 1800    | 3.27 | 3.899 | 3.339 | 3.911 | 3.465 |
| 2000    | 3.827 | 4.355 | 3.838 | 4.632 | 4.035 |

| E/N(Td) | Xe | Ne | Kr | He | Ar |
|---------|----|----|----|----|----|
| 100     | 5.763 | 11.81 | 7.375 | 9.916 | 8.659 |
| 200     | 5.52 | 11.27 | 6.874 | 9.551 | 8.062 |
| 300     | 5.35 | 10.79 | 6.469 | 9.231 | 7.547 |
| 400     | 5.236 | 10.34 | 6.134 | 8.947 | 7.1 |
| 500     | 5.154 | 9.925 | 5.85 | 8.693 | 6.757 |
| 600     | 5.1 | 9.531 | 5.607 | 8.465 | 6.388 |
|   |     |     |     |     |     |     |     |     |     |
|---|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| 700| 5.066| 9.157| 5.398| 8.265| 6.074| 5.298| 12.94| 6.01| 1.179| 6.482|
| 800| 5.051| 8.806| 5.218| 8.101| 5.585| 5.5661| 12.35| 5.912| 1.199| 6.299|
| 900| 5.053| 8.482| 5.063| 7.99| 5.654| 5.458| 11.79| 5.836| 1.235| 6.176|
| 1000| 5.076| 8.192| 4.93| 7.959| 5.5| 5.585| 11.26| 5.779| 1.277| 6.119|
| 1200| 5.124| 7.937| 4.822| 8| 5.418| 5.74| 10.72| 5.731| 1.31| 6.13|
| 1400| 5.195| 7.703| 4.739| 8.08| 5.38| 5.903| 10.17| 5.678| 1.322| 6.205|
| 1600| 5.277| 7.462| 4.681| 8.141| 5.4| 6.043| 9.588| 5.593| 1.307| 6.322|
| 1800| 5.339| 7.184| 4.63| 8.09| 5.452| 6.109| 8.976| 5.454| 1.269| 6.44|
| 2000| 5.34| 6.851| 4.564| 7.9| 5.477| 6.066| 8.348| 5.48| 1.218| 6.512|
Figure(1). The electron energy distribution function versus the electron energy for pure CF3I and mixture with noble gaseous (50/50%).
Figure (2). The electron mean energy as a function of E/N in various mixture of CF₃I with Noble gases (Ar, He, Kr, Ne and Xe).
Figure (3). The density–normalized mobility as a function of $E/N$ in various mixture of CF$_3$I with Noble gases (Ar, He, Kr, Ne and Xe).
Figure (4). density–normalized longitudinal diffusion coefficient as a function of $E/N$ in various mixture of CF$_3$I with Noble gases (Ar, He, Kr, Ne and Xe).
Figure (5). density –normalized longitudinal diffusion coefficient as a function of E/N of pure CF$_3$I.

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