Electron transport coefficients and negative streamer dynamics in CF_3I-SF_6 mixtures

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***Abstract*—A multi term theory for solving the Boltzmann equation and a Monte Carlo simulation technique are used to calculate electron transport coefficients in the mixtures of CF_3I and SF_6 as a function of the applied electric field. The calculated transport coefficients are then used as an input in the fluid equation based models to investigate the transition from an electron avalanche into a streamer and streamer propagation. Electron transport coefficients are also calculated in radio-frequency electric and magnetic fields crossed at arbitrary phases and angles. A multitude of kinetic phenomena induced by the synergism of the magnetic field and electron attachment is observed and discussed using physical arguments.**

Keywords—Boltzmann equation, Monte Carlo, transport coefficients, streamers, electron attachment, ionization

I. Introduction

Studies of electron transport processes in strongly attaching gases in electric and magnetic fields have many important applications. These applications range from the modelling of magnetically-assisted low-pressure collision dominated plasma discharges to the modelling of gaseous particle detectors in high-energy physics and to the development of a new generation of gaseous dielectrics in high-voltage technology. In the present work, we are investigating the electron transport and the streamer propagation in the mixtures of strongly attaching gases trifluoroiodomethane (CF_3I) and sulfur hexafluoride (SF_6). In high-voltage technology, strongly attaching gases and their mixtures with other appropriate gases such as N_2 and/or CO_2 are used with the aim of controlling and preventing the electrical breakdown in electric power systems. The most important gaseous dielectric in high voltage technology nowadays is SF_6. SF_6 is a strongly attaching gas, with a high dielectric strength, and a breakdown voltage nearly three times higher than that of air at atmospheric pressure. However, in electrical discharges, SF_6 creates highly toxic and corrosive compounds such as S_2F_{10} and SOF_2. In addition, SF_6 has an extremely high global warming potential (23900 times higher than that of CO_2) and an extremely long atmospheric lifetime (3200 years) [1]. These facts have moved physicists and engineers into finding possible substitutes of SF_6. One of the most promising candidates is CF_3I. CF_3I is also a strongly attaching gas, but with much higher dielectric strength than SF_6. The global warming potential of CF_3I is much less than that of SF_6 (approximately 0.4 times that of CO_2), and its lifetime in the atmosphere is very short (1.8 days). Using these facts as motivational factors, we have undertaken a program to understand electron interactions with CF_3I as well as the basic properties of electron transport and streamer propagation in pure CF_3I and its mixtures with SF_6.

In the present investigations, we have calculated electron transport coefficients in various mixtures of CF_3I and SF_6 subjected to an external static electric field. Our results are based on a numerical multi term solution of the Boltzmann equation [2,3], which is solved for values of E/N ranging from approximately 50 to 10 000 Td (1 Td = 10^{-21} Vm^2). For the lower values of E/N, due to poor convergence of transport coefficients we have applied the Monte Carlo method. The Monte Carlo code has been recently optimized and specified to consider the transport processes of electrons in strongly attaching gases [4]. The poor convergence of transport coefficients is a consequence of predominant removal of the lower energy electrons due to a strong electron attachment, which in turn shifts the bulk of the distribution function towards a higher energy. Under these conditions, the moment method for solving the Boltzmann equation used in the present work usually fails, as it requires a prohibitive number of basis functions for resolving the energy dependence of the distribution function.

Calculations have also been performed in the case of alternating current (ac) electric and magnetic fields. We investigate the way in which the transport coefficients and other swarm properties are influenced by the field frequency, electric and magnetic field strengths, and the phase difference between the fields under conditions in which the electron transport is greatly affected by electron attachment. The time-dependent behavior of electron swarms in varying configurations of electric and magnetic fields is particularly important for the modeling of magnetically controlled/assisted radio-frequency plasma discharges [3]. In addition, the time-dependent studies are useful for a future development of sensors for detection of electromagnetic waves induced in gas-insulated high-voltage switchgear (GIS) by partial discharges.

Finally, the calculated transport coefficients in a direct current (dc) electric field are used as an input in the fluid-equation based models with the aim of investigating the transition from an electron avalanche into a streamer and

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streamer propagation. Among many important points, in the present work we discuss how streamer properties, including the electron density, electric field and streamer velocity are affected by introducing CF_3I into SF_6.

II. Theoretical Method

The behavior of electron swarms in neutral gases under the influence of electric and magnetic fields is described by the phase-space distribution function $f(\boldsymbol{r},\boldsymbol{c},t)$, representing the solution of the Boltzmann equation

$$\frac{\partial f}{\partial t}+\boldsymbol{c}\cdot\frac{\partial f}{\partial \boldsymbol{r}}+\frac{e}{m}(\boldsymbol{E}+\boldsymbol{c}\times\boldsymbol{B})\cdot\frac{\partial f}{\partial \boldsymbol{c}}=-J(f,f_0)\,, \qquad (1)$$

where $\boldsymbol{r}$, and $\boldsymbol{c}$ denote the position and velocity coordinates respectively, while e and m are the charge and the mass of the swarm particle and t is the time. The right-hand side $J(f,f_0)$ denotes the linear electron-neutral molecule collision operator, accounting for elastic, inelastic and non-conservative collisions. The electric and magnetic fields are assumed to be spatially-homogeneous and in the general case time-dependent.

The methods and techniques for solving the Boltzmann equation are by now standard and the reader is referred to our previous works [3,4]. Nevertheless, we highlight some important steps of our methodology for solving the Boltzmann equation:

1) No assumptions on symmetries in velocity space are made, and the directional dependence of $f(\boldsymbol{r},\boldsymbol{c},t)$ in velocity space is represented in terms of a spherical harmonic expansion:

$$f(\boldsymbol{r},\boldsymbol{c},t)=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}f(\boldsymbol{r},\boldsymbol{c},t)Y_m^{[l]}(\hat{\boldsymbol{c}})\,, \qquad (2)$$

where $Y_m^{[l]}(\hat{\boldsymbol{c}})$ are spherical harmonics, and $\hat{\boldsymbol{c}}$ represents the angles of $\boldsymbol{c}$. In contrast to the frequently used two-term approximation which forms the basis of the classical theory of electron transport in gases, our method is a truly multi-term approach. The differences between the two-term approximation and our multi-term approach for solving the Boltzmann equation will be illustrated for electron transport in CF_3I in the next section.

2) Under hydrodynamic conditions (far away from the boundaries, sources and sinks of electrons) a sufficient representation of the space dependence is an expansion of $f(\boldsymbol{r},\boldsymbol{c},t)$ in terms of the powers of the density gradient operator:

$$f(\boldsymbol{r},\boldsymbol{c},t)=\sum_{k=0}^{\infty}f^{(k)}(\boldsymbol{c},t)\odot(-\nabla)^k\,n(\boldsymbol{r},t)\,, \qquad (3)$$

where $f^{(k)}(\boldsymbol{c},t)$ are time-dependent tensors of rank k while $\odot$ denotes a k-fold scalar product.

3) The energy dependence of $f(\boldsymbol{r},\boldsymbol{c},t)$ is represented by an expansion about a variety of Maxwellians at an arbitrary temperature in terms of Sonine polynomials.

The combination of spherical harmonics and Sonine polynomials yields the well-known Burnett functions. Using the appropriate orthogonality relations of the Burnett functions, the Boltzmann equation is converted into a hierarchy of doubly and infinite coupled inhomogeneous matrix equations for the time-dependent moments. The finite truncation of the Burnett functions, permits a solution of this hierarchy by direct numerical inversion. These equations are solved numerically and both families of transport coefficients, the bulk and the flux, including other transport properties, are expressed in terms of moments of the distribution function [2,3].

In addition to Boltzmann's equation, in the present work we apply a Monte Carlo simulation technique. Our standard MC code has been recently extended to consider the spatially inhomogeneous electron swarms in strongly attaching gases by implementing the rescaling procedures [4]. The so-called discrete and continuous rescaling procedures are developed and benchmarked in the aim of simulating electron transport under conditions of extensive losses of seed electrons due to a strong electron attachment. In this work, Monte Carlo method is employed as a tool to confirm the numerical accuracy and integrity of a multi-term theory for solving the Boltzmann equation. However, whenever the convergence of transport coefficients was poor in the Boltzmann equation analysis, then MC results are in turn included in the plots.

Transition from an avalanche into a streamer, and propagation of streamers have been considered by the fluid equation based models. We employ the so-called classical fluid model in which the equation of continuity is combined with the drift-diffusion approximation. The resulting equation is coupled with the Poisson equation for the space charge electric field calculations. The resulting system of partial differential equations is solved numerically assuming the local field approximation [5,6].

III. Results and Discussion

A. Cross sections and inputs

The development of the complete cross-section set of electron scattering in CF_3I has been detailed in recent studies [4,7], and is based largely on the original set proposed by Kimura and Nakamura [8]. The accuracy and the completeness of the initial set developed by Kimura and Nakamura was improved by applying the standard swarm procedure using the measurements of transport coefficients in the mixtures of CF_3I with Ar and CO_2 under the pulsed-Townsend (PT) conditions. Cross sections for electron scattering in SF_6 are taken from Itoh et al. [9]. In the present investigation, we consider the density-reduced electric field range from 1 to 10^4 Td. The background gas mixture temperature is fixed at 293 K. In the domain time-dependent studies, we cover a range of magnetic field amplitudes between 0 and 10^4 Hx (1 Hx = 10^{-27} Tm^{-3}).

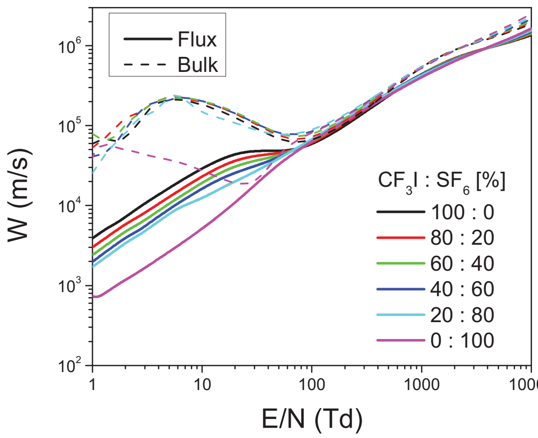

Fig. 1. Variation of the flux and bulk drift velocities with E/N for various CF_3I-SF_6 mixtures.

B. Transport coefficients in the mixtures of CF_3I and SF_6

In Fig. 1 we show the variation of the flux and bulk drift velocities with E/N for various CF_3I-SF_6 mixtures. We observe that over the entire range of E/N the flux drift velocity is a monotonically increasing function of E/N, while the bulk drift velocity in pure CF_3I and SF_6, as well as in their mixtures, exhibits a pronounced negative differential conductivity (NDC). NDC is characterized by a decrease in the bulk drift velocity despite an increase in the magnitude of the applied electric field. In the case of strongly attaching gases such as CF_3I and SF_6, NDC is induced by the combined effects of attachment heating and inelastic cooling of the swarm. In addition, due to attachment heating and explicit effects of ionization, the bulk drift velocity dominates the flux component over the entire range of E/N considered in this work.

In Fig. 2 we show the variation of the ionization and attachment rate coefficients with E/N for various mixtures. As expected, the ionization rate coefficient is a monotonically increasing function of E/N and becomes significant at the higher values of E/N when sufficient electrons have enough energy, to cause ionization. We observe that the ionization rate is less sensitive with respect to the composition of the gas mixture at higher values of E/N. The behavior of the attachment rate coefficient is more complex, but generally it tends to decrease with increasing E/N.

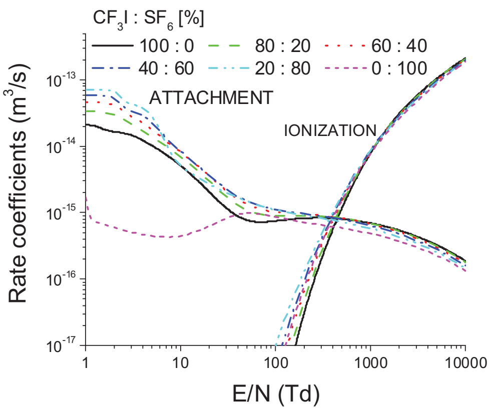

Fig. 2. Variation of the attachment and ionization rate coefficients with E/N for various CF_3I-SF_6 mixtures.

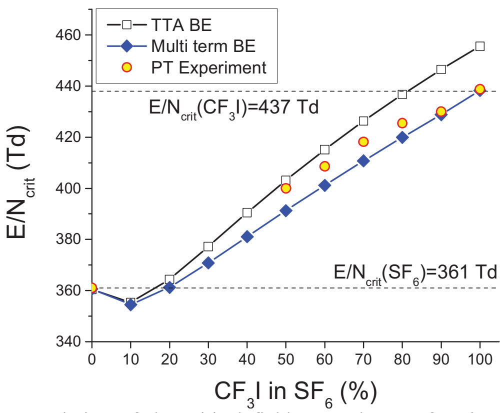

Fig. 3. Variation of the critical field strength as a function of the CF_3I content in the CF_3I-SF_6 mixture. Results obtained by the two-term approximation (TTA) and multi-term approach for solving the Boltzmann equation are compared with the measurements under the PT conditions.

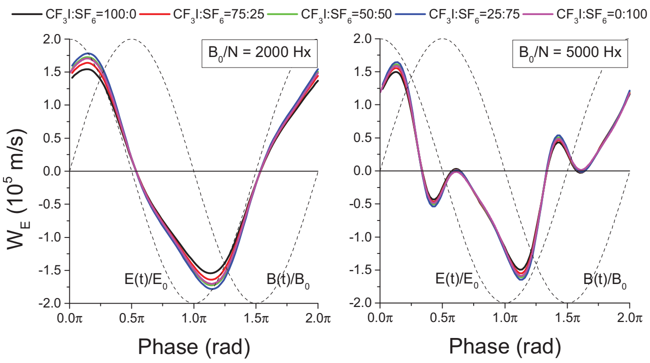

Fig. 4. Temporal profiles of the flux drift velocity for various CF_3I-SF_6 mixtures. The electric field amplitude is 350 Td and the field frequency is 1000 MHz.

In Fig. 3 we show the variation of the critical electric field (or limited electric field) as a function of the per cent content of CF_3I in the mixture. The critical electric field is a value of E/N for which rate coefficients of electron attachment and ionization are equal. This property is of great importance not only in studies of low-current dc discharges and streamers, but may also be useful for studies of some rf discharges. The results obtained by solving the Boltzmann equation are compared with the measurements under the PT conditions. Our multi term results and measurements agree very well for the pure gases. We observe that the TTA significantly overestimates the measurements and multi-term results for pure CF_3I.

C. Transport coefficients in radio-frequency electric and magnetic fields

In Fig. 4 we show the temporal profiles of the longitudinal flux drift velocity for various CF_3I-SF_6 mixtures. Calculations are performed in a crossed field configuration while the phase difference between the electric and magnetic fields is set to π/2 rad. The magnetic field amplitudes are 2000 Hx (left panel) and 5000 Hx (right panel). We observe that the profiles are asymmetric and phase-delay of the W_E curves relative to the electric field is clearly evident due to temporal non-locality [4]. The maximum values of W_E are dependent on the gas composition. The time-averaged power absorbed by the swarm (or plasma or any active medium) is given by:

$$\langle p_{abs} \rangle = \frac{1}{T}\int_0^T -eN_0 \boldsymbol{W}(t) \cdot \boldsymbol{E}(t) dt \,, \qquad (4)$$

where N_0 is the number of electrons in the swarm, T=2π/ω is the period, $\boldsymbol{W}$ is the time-dependent average velocity and $\boldsymbol{E}$ is the time-dependent electric field. From Eq. (4), it is clear that the phase difference between the drift velocity and electric field controls the power absorption: (i) when the drift velocity $\boldsymbol{W}$ and electric field $\boldsymbol{E}$ have the same sign, the instantaneous power is positive, and (ii) when the drift velocity $\boldsymbol{W}$ and electric field $\boldsymbol{E}$ have the opposite sign, then the instantaneous power is negative. This suggests that when the power is positive the electric field pumps the energy into the system while when the power is negative the energy is transferred from an active medium to the external circuit.

In Fig. 5 we show the variation of the cycle-averaged power as a function of the magnetic field amplitude for various CF_3I-SF_6 mixtures. We observe that the absorbed power depends on the gas composition. One of the most striking phenomena is the presence of periodic structures in the profile of the absorbed power. Comparing CF_3I and SF_6, these structures are more pronounced for CF_3I. For dc electric and magnetic fields the absorbed power is always a monotonically decreasing function of the applied magnetic field, while in this case we may observe a multitude of peaks in the B_0/N-profiles of this property. This is a clear sign of the resonant absorption of energy from the rf electric and magnetic fields. We see that these effects are more pronounced for the lower values of B_0/N, where on the average the electrons only complete partial orbits between collisions.

D. Transition from an electron avalanche into a negative streamer its propagation in the CF_3I-SF_6 mixtures

In Figs. 6 (a) and (b) we show the temporal evolution of the electric field and electron density, respectively for various CF_3I-SF_6 mixtures. Calculations are performed in a 1-dimensional setup. The initial Gaussian grows due to the ionization and then charge separation occurs due to the drift of positive ions in the opposite direction. As a consequence, the initial homogeneous electric field is disturbed and the field in the ionized region becomes more and more screened. Due to space charge effects the electric field drops off to the level in which ionization stops and only attachment occurs. As a consequence, the electron density in the streamer channel is significantly reduced. By mixing CF_3I with SF_6, the streamers become slower and the screening of the externally applied electric field is less pronounced.

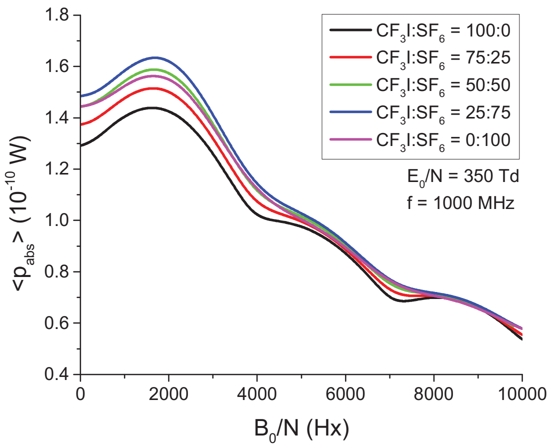

Fig. 5. Variation of the cycle-averaged power of electrons for various CF3I-SF6 mixtures. The electric field amplitude is 350 Td and the field frequency is 1000 MHz.

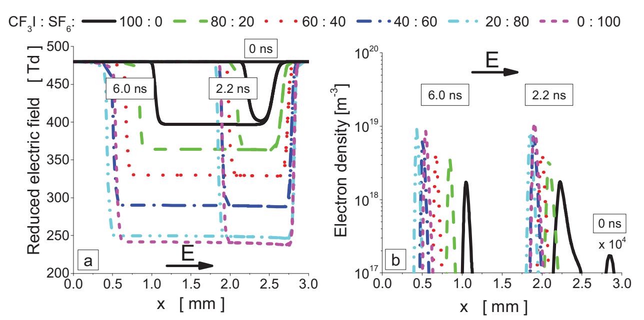

Fig. 6. Temporal evolution of the electric field (a) and electron density (b) in a planar front in various CF_3I-SF_6 mixtures. The externally applied electric field is 480 Td and streamers move from the right to the left.

IV. Conclusion

In this paper, we have used a multi term theory for solving the Boltzmann equation and a Monte Carlo simulation technique to investigate electron transport in the mixtures of CF_3I and SF_6. From the point of view of a possible application of CF_3I and its mixtures with SF_6 as gaseous dielectrics, we have calculated the drift velocity, rate coefficients for electron attachment and ionization and critical electric field. The previous studies [10] are extended by considering the duality of transport coefficients, e.g. the existence of two different families of transport coefficients, the bulk and the flux. Comparing the bulk and flux drift velocities, it is found that the bulk component shows a very strong NDC and behaves in a qualitatively different fashion. Calculations in dc electric fields are augmented by those in rf electric and magnetic fields. We have paid a particular attention to the power absorption of the swarm. Due to a complex interplay of the effects induced by temporal non-locality, magnetic field and cyclotron resonance, we have observed a multitude of peaks in the B_0/N profiles of the absorbed power. Finally, using the classical fluid model we have simulated the transition from an electron avalanche into a negative streamer. It is shown that streamers in the mixtures with a higher content of CF_3I are slower, the electron density is reduced and the electric field in the streamer interior is enhanced. Thus, by mixing CF_3I with SF_6, the insulation characteristics of the mixtures are considerably improved.

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