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NUMERICAL ANALYSIS OF DISCHARGE MECHANISMS IN SF₆ USING THE MONTE CARLO METHOD

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Abstract: Sulphur hexafluoride (SF₆) is extensively used in the field of electric power apparatus and high voltage engineering because of its high dielectric strength. The electron swarm parameters in attaching gases have several applications. It is important for gaseous insulation in power apparatuses, for optimisation of gaseous insulating systems and the application of plasma to understand the mechanisms of the electric discharge processes in gases. However, the calculation of physical parameters for the electrical discharges is very difficult and complicated; numerical simulation of transport parameters of charged particles and the development processes for streamer and corona discharges in gas is used. The present work is to analysis the electron swarm parameters and the electric field characteristics of streamer and corona discharges using a kinetic method. The electric discharge properties in SF₆ gas, the initiation and propagation of the streamer and corona discharge in a highly non-uniform electric field as function of the time were studied. The electron transport parameters in SF₆ were calculated by the Monte Carlo method.

Keywords: Monte Carlo simulation; transport parameters; Discharge; SF₆; Streamer; Corona.

1 Introduction

There are a lot of applications of the streamer and corona discharges like the surface treatment, water treatment, treatment of gaseous pollutants, and medical applications. The streamer discharge is the first processes of the dielectric breakdown. The initiation and propagation of streamer discharge has a significant importance for these processes, which implicate to understand the fundamental physics of the streamer discharge. Physical plasmas and its applications is a key technology for different activities, like the aerospace, automotive, biotechnology, and others industries. In the medical treatment with the plasma it is important to know the energy of charged particles, the chemical processes and the interactions of these particles with the biological matter [1-7]. For optimization and development the technologies of plasma applications it is necessary to understand the fundamental processes of electrical discharges and knowledge the particles charged parameters in plasma. The properties of electron transport play a necessary role in the simulation of the chemical processes in the plasmas. Simulation of the

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electron transport parameters and discharges is necessary to understanding the effects in the applications and potentials applications of plasma. For understanding the different processes in the electrical discharges and dielectric breakdown in the gases it is crucial to know the electron swarm parameters in these gases [8-16]. For these fields the studies of the electrical discharges are a high importance. Knowledge the electron swarm parameters are great importance for simulating the initial development and propagation of the electric discharge. The characteristics of streamer discharge and corona discharge oblige us to study the process of the kinetics phenomenon in these discharges. The sulphur hexafluoride (SF_6) is an electronegative gas; for that it has an outstanding insulating property, the breakdown strength higher than air at atmospheric pressure, it is a very stable, is chemically inert, nonflammable gas, and nontoxic. For these excellent characteristics the SF_6 is used in the high voltage equipments, power production, distribution, electric transmission. Especially of the properties of the electronegative gases, the SF_6 is frequently used in the applied of the plasma for the nanotechnology and also in the plasma processing technologies. [17-21]. The investigations were made on these physicals phenomena with the kinetic Monte Carlo method to simulate the electron swarm parameters, electron avalanches, streamer discharge and corona discharge with the initiation and developments of electric discharge in SF_6 gases. Monte Carlo simulation of electron transport parameters has the advantage that the motion of the charged particles in the discharge is traced in the time and in the space.

2. Method of the model and procedures With the Monte Carlo technique we can simulate a process in hydrodynamic and in non-hydrodynamic regimes [22]. The Monte Carlo method enables us to simulate the charged particles transport in gases under the influence of the electric field from an initially number of charged particles. These particles are followed until the limits of the domain of the simulation or their disappearance by collision processes. The electron collision cross sections define the probability of the elastic, or inelastic collisions of the electron with molecules of gas. The information on the primary and secondary electrons (space, velocity, etc.) is saved in a file so to calculate the transport parameters and the electric field. Whether a collision between an electron and a gas molecule occurs or not is decided by generating a random number uniformly distributed between 0 and 1 [23]. For the simulation of the transport parameters, a background gas of SF_6 molecules with a number density of $N=3.29 \cdot 10^{22} \text{ m}^{-3}$ at 20°C in a spherical coordinate system is considered. A unit of $1\text{Td} = 10^{-21} \text{ V} \cdot \text{m}^2$ is used to avoid a large negative powers of 10. It is difficult to determine the microscopic parameters of streamer discharges by experiments due to the complex of the processes, unforeseeable displacement and unknown directions of propagation. Monte Carlo method is a practical method to simulate the collisions of electrons with SF_6 and the growth of an avalanche. From the origin of the coordinate system an Initial electrons with a constant energy are injected assuming a cosine distribution for the angle of entry, the electric field is anti-parallel to the z-axis. In the Monte Carlo technique to simulate the streamer discharges we include the photoionization process. [24, 25]. Understanding of the physical process of the corona discharge is very complicated, because of the presence of nonuniform electric field this makes difficult to calculate the probabilities of collision in inter electrodes space. With the Monte Carlo technique we can take into account the distortion of the electric field by the space charge. The corona discharge is represented by two areas, close to the active electrode surface a thin zone, called ionization zone, and toward the plate electrode a drift zone, for any shape or type of ionizing electrode. The initial electrons are emitted from the cathode according to a cosine distribution, and the electric field is anti-parallel to the z-axis. The simulation also included the photoionization process. [26, 27]

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3. Results and discussion

The fabrication processes by plasmas, developments and applications of high voltage devices demand the investigations on the fundamental physics that occur in the discharges. Consequently the calculations of the charged particles swarms and electron transport parameters are essential to modelling and simulating of the phenomena occurring in these processes. In the Monte Carlo simulation we have injected 10000 electrons to avoid fluctuations for low values of the reduced electric field (E/N). At $t=0$ and $r=0$ with a cosine distribution the first electrons are injected with a energy of 0.1 eV, we chose this low energy so as not to influence the electron transport parameters at later times. In Fig. 1, Fig. 2, Fig. 3 and Fig. 4 showing the variation of electron drift velocity and electron energy with time, and the ionization and attachment coefficients with time for different reduced electric field values. Some time is needed for drift velocity, electron mean energy and ionization coefficient to reach the steady states. With the time the electron attachment coefficient decreases, because of high electron attachment cross section of the SF_6 gas for the low energies. In SF_6 , the high electron attachment cross section makes the electron attachment process by sulfur hexafluoride higher and increases the insulation performance. Near the ionization threshold in the electron cross section of the sulphur hexafluoride, the collisions of electrons with the SF_6 molecules can produce electrons with low energies and caused the attachment process. When the reduced electric field increases the ionization coefficient increases and the attachment coefficient decreases. We notice that the electron ionization coefficient exceeds the electron attachment coefficient for the reduced electric field of 500 Td and more. Application of the Monte Carlo to calculate the electron swarm parameters in the range of 100-1000 Td is obtained. The tendencies of the electron drift velocity and electron energy in the SF_6 , as the reduced electric field increases, are characterized as shown in Fig. 5 and Fig. 6. The curves of electron drift velocity and the electron energy in function of the reduced electric field have a growing trend with E/N . As shown in Figures 7 and 8 the reduced ionization and reduced attachment coefficients are according to the reduced electric field. The reduced ionization coefficient increases with the reduced electric field, however that the reduced attachment coefficient decreases with the increase of the reduced electric field. The electron reduced ionization coefficient α/N of SF_6 increases with the increase in the reduced electric field. The electron reduced attachment coefficient η/N of SF_6 decreases with the increase in E/N . With the increase of the reduced electric field the number of ionization of the SF_6 molecules increases and the probability of the attachment process is reduced. The electron energy distribution at the reduced electric field $E/N=800$ Td is shown in Fig. 9. The dot and full lines show the Maxwellian distribution at the same energy. The distribution with the anisotropic parts is much greater than with isotropic part alone. This is due to the fluctuation resulting from the acceleration of electrons between two collisions. It is important to know the characteristics and the properties of the electrical discharges and the swarm parameters in gases are necessary to develop the technological applications. With the use of the electron collision cross section of the SF_6 , the electron transport parameters are calculated by the Monte Carlo technique, a good agreement is obtained between the measured and calculated values. The results obtained by the Monte Carlo technique for the electron transport parameters for the SF_6 show that simulation with this method gives of good results

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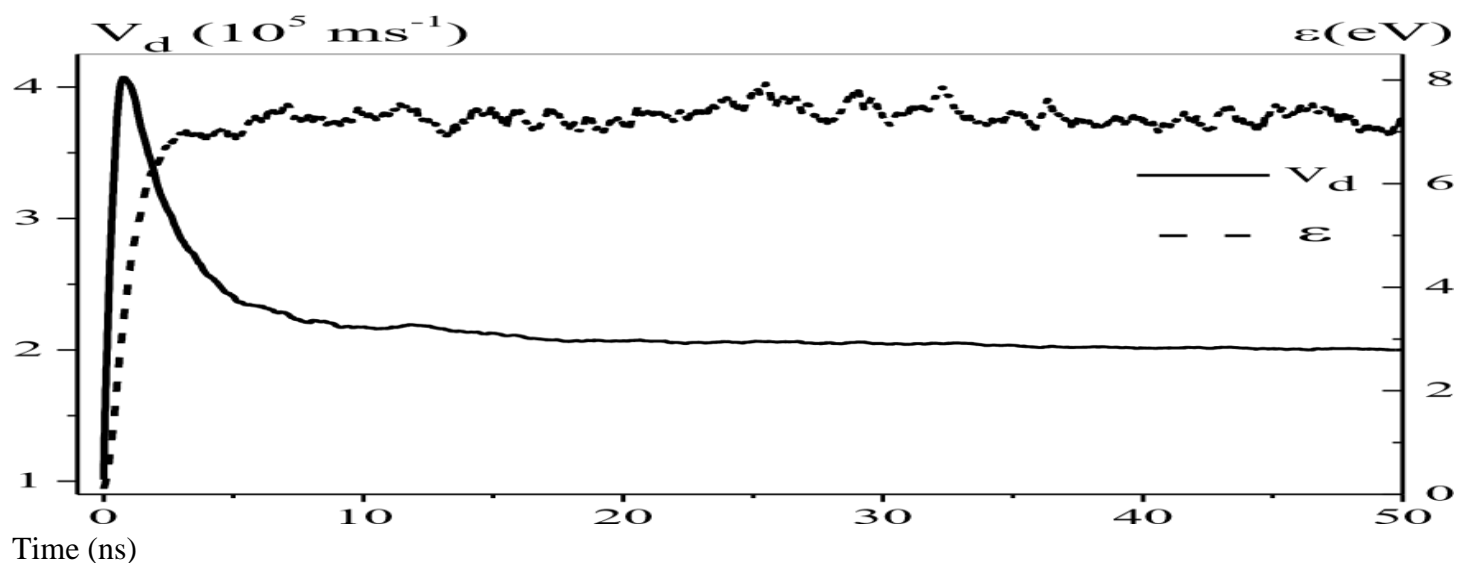


Fig. 1. Electron Drift velocity (W) and electron main energy (\square) for 300 Td

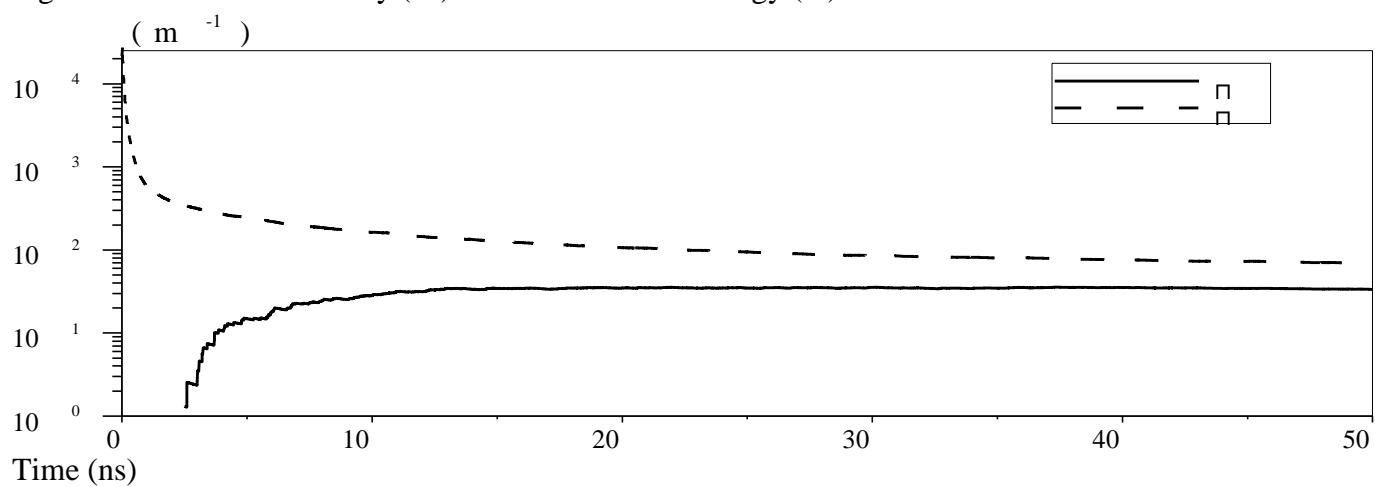


Fig. 2. Ionization (\square) and attachment (\square) coefficients for 300 Td

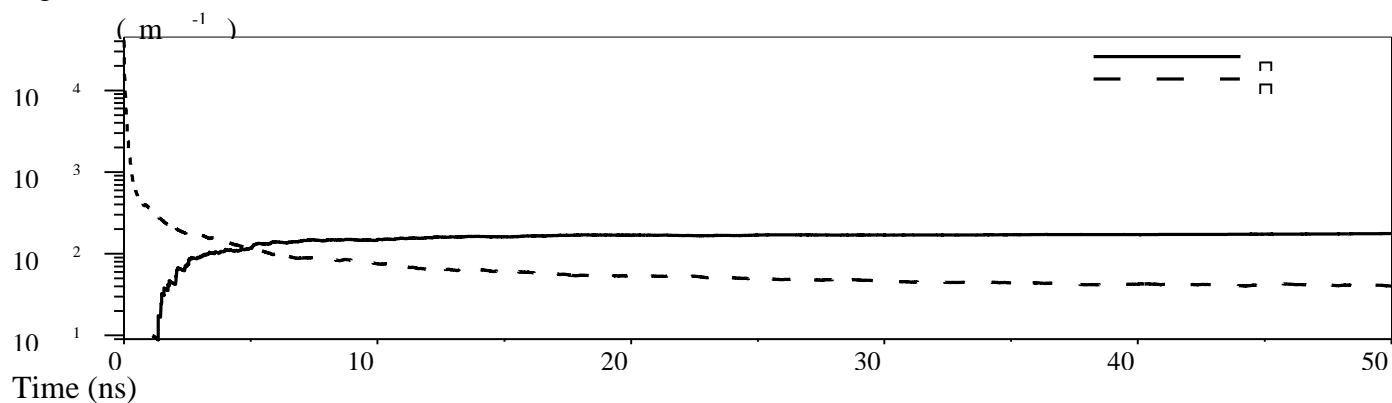


Fig. 3. Ionization (\square) and attachment (\square) coefficients for 500 Td

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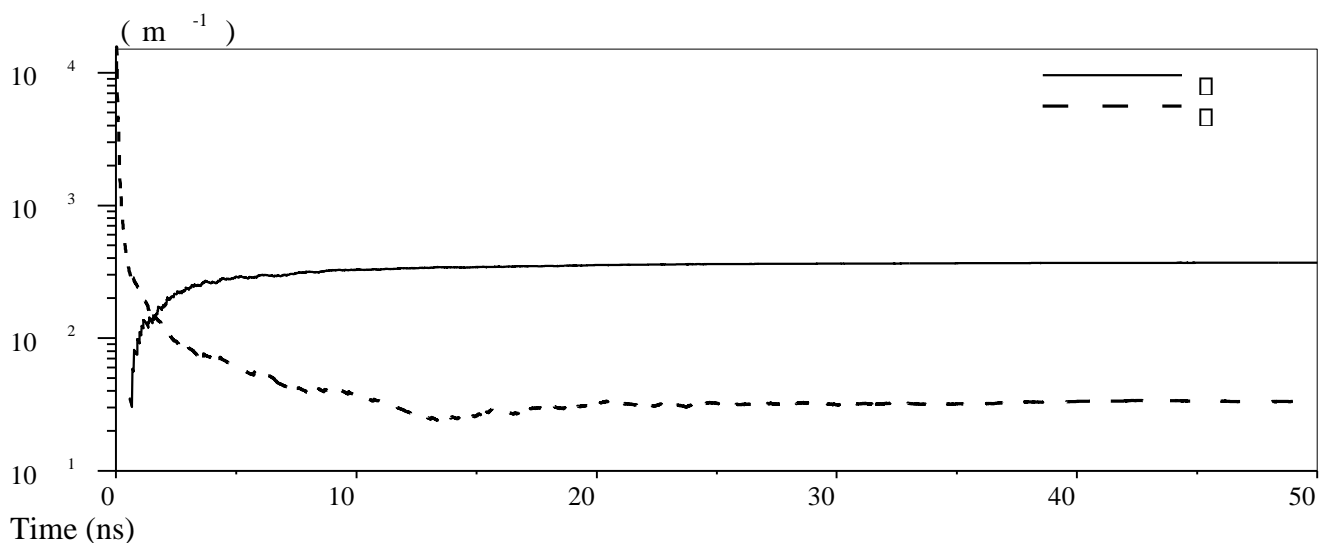


Fig. 4. Ionization (\square) and attachment (\square) coefficients for 700 Td

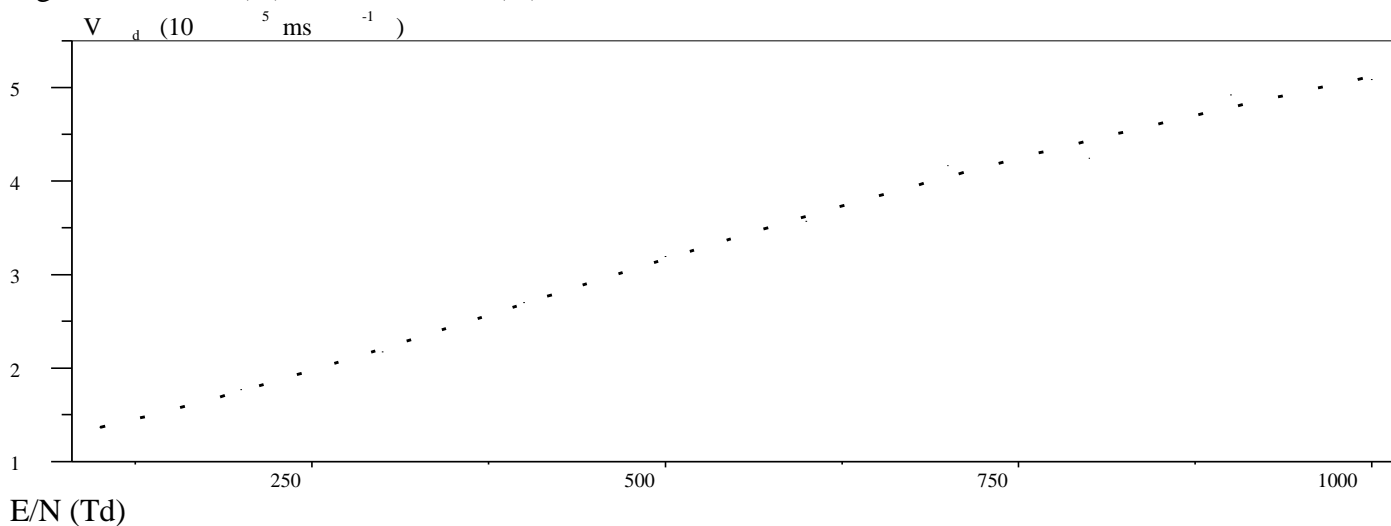


Fig. 5. Electron drift velocity

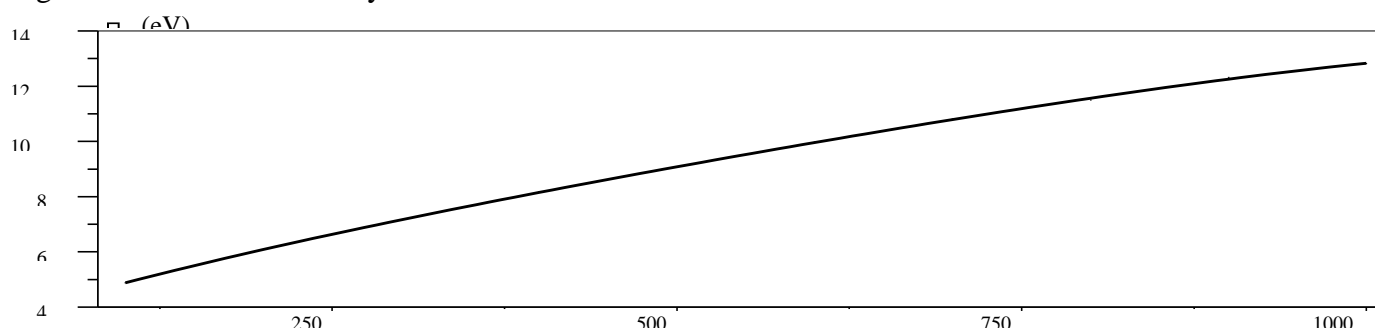


Fig. 6. Electron main energy

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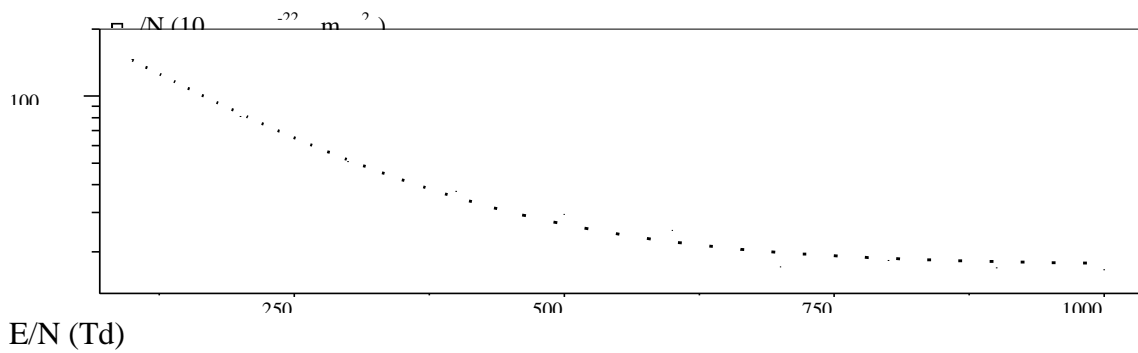


Fig. 7 Reduced attachment coefficient

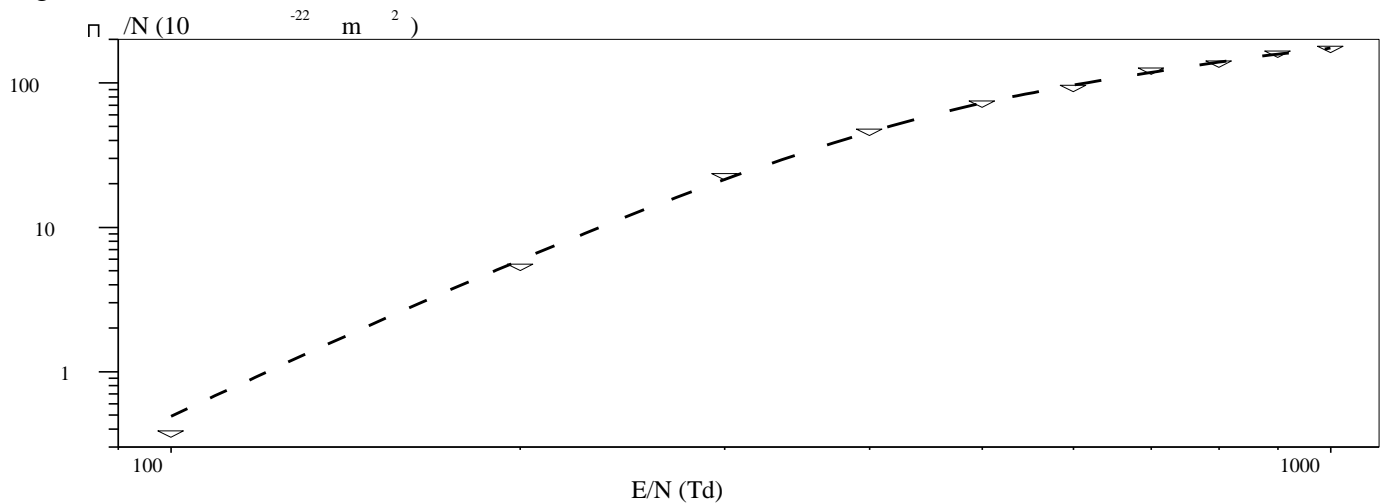
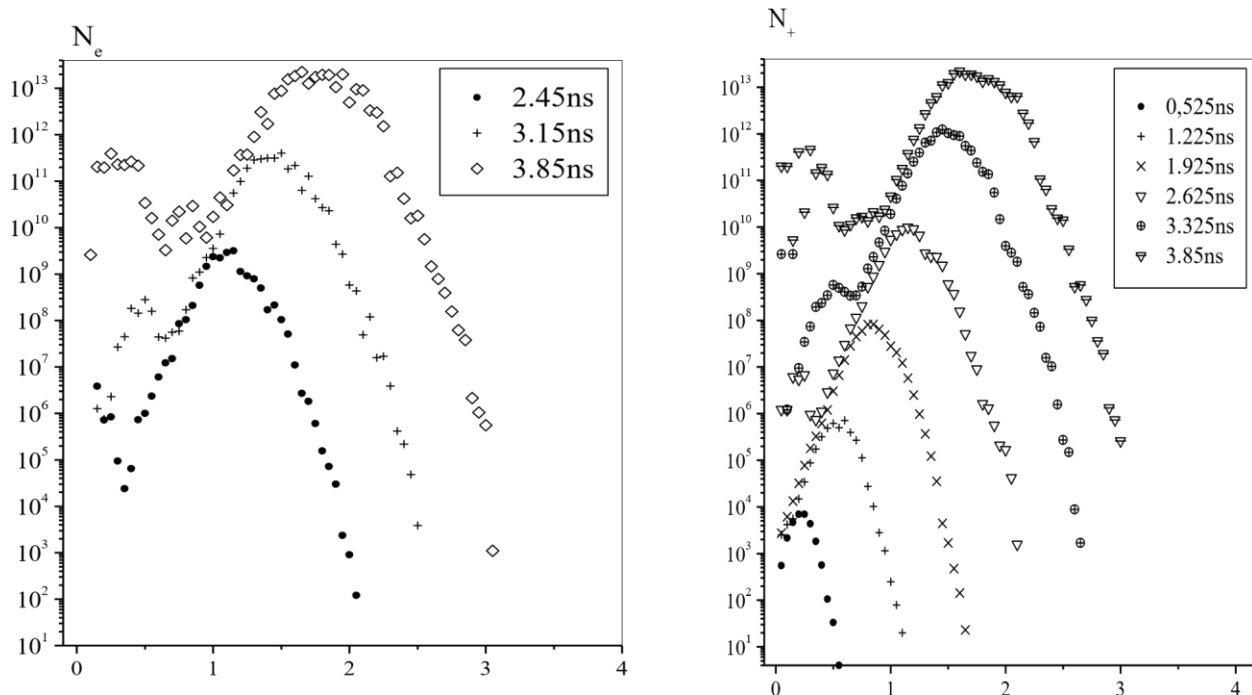


Fig. 8 Reduced ionization coefficient

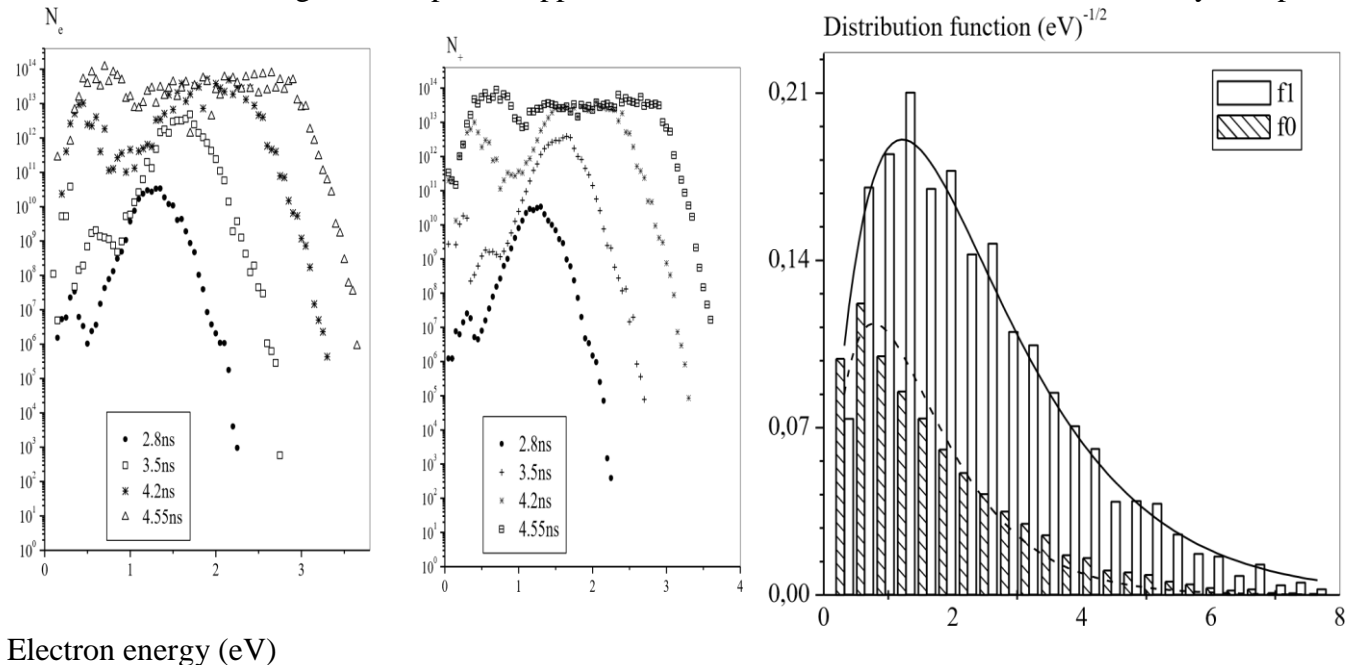
In the engineering the electrical discharges in the gases are very used in industries, this implies the utility of the

studies
of
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swarm



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parameters: the main energy, drift velocity, ionization and the attachment coefficients. For studying the macroscopic and physical properties of the electrical discharges and plasma, the modelling and simulation of the electron swarm parameters and the formation and propagation of the electron avalanches are essential to understand the important process in the gas discharge and plasma. In the high voltage power transmission the SF₆ gas is an important insulation; it is important to know the electrical discharge process and the electron transport parameters. With the Monte Carlo simulation we calculate the number of the charged particles and the initiation of the avalanches and propagation of the streamer and corona discharges. The Monte Carlo simulation method is used to simulate the phenomenon of initiation and propagation of the streamer and corona discharges characteristics. In the initial of the simulation without an external electric field, there are a few electrons in SF₆. When an electric field is applied, the number of the electrons and ions increases the reason of that is the ionization, attachment, excitations and vibrations, and elastic reactions. This simulation allows us to follow the spatiotemporal evolution of the electrons, positive and negative ions in the SF₆ gas, and the spatiotemporal characteristics of the electric field along the development and propagation of the streamer and corona discharges. The streamer discharge and the corona discharge in gas create particles and chemical reactions. For several applications the processes generated by the streamer discharge and the corona discharge in gas are utilized. These discharges develop in an applied electric field with the electric field created by the space charge.



Electron energy (eV)

Fig. 9 Electron energy distribution at E/N=800 Td, f0: isotropic part, f1: with anisotropic parts.

Distance (mm)

Fig. 10 Evolution of electron density

Distance

(Mm)

Fig. 11 Evolution of electron density

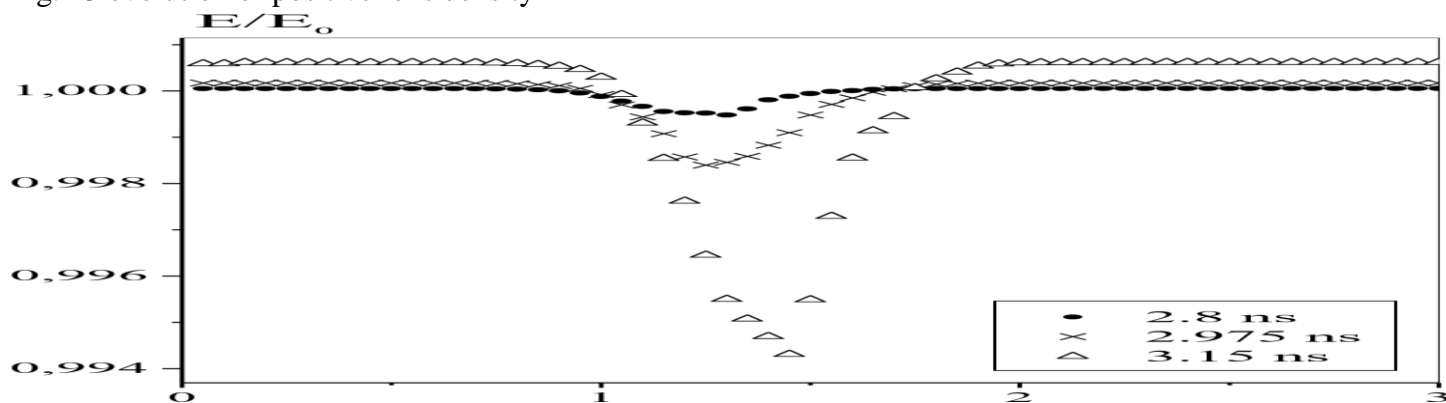
Distance (mm)

Fig. 12 evolution of positive ions density

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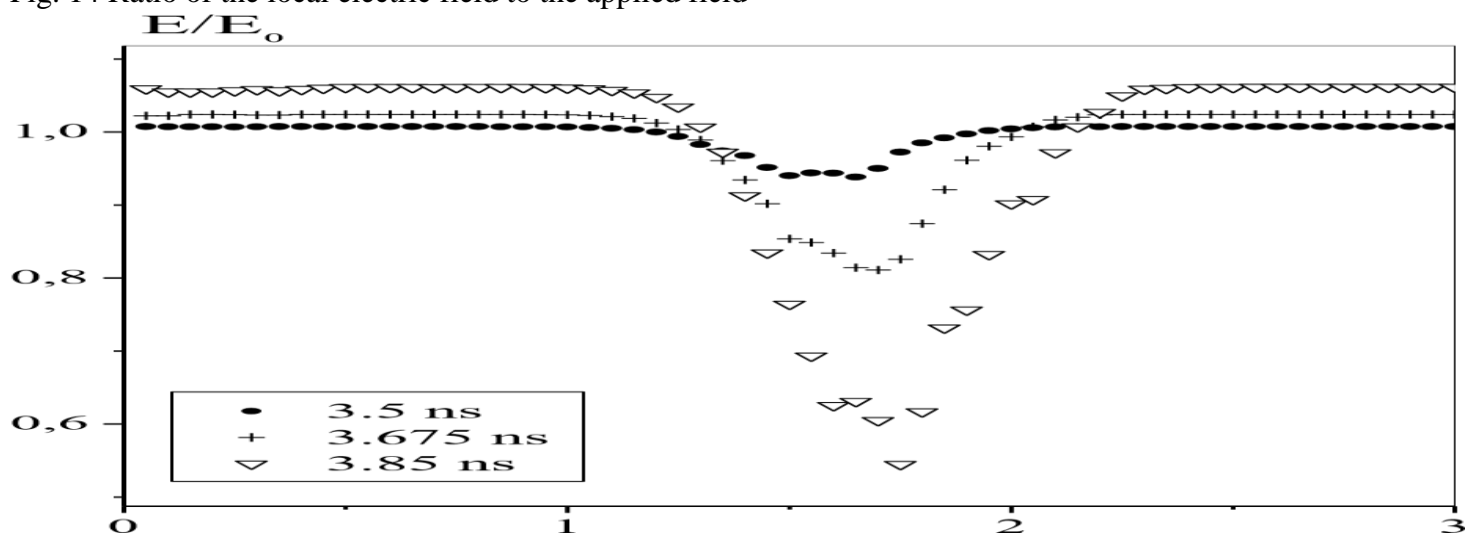
Distance (mm)

Fig. 13 evolution of positive ions density



Distance (mm)

Fig. 14 Ratio of the local electric field to the applied field



Distance (mm)

Fig. 15 Ratio of the local electric field to the applied field

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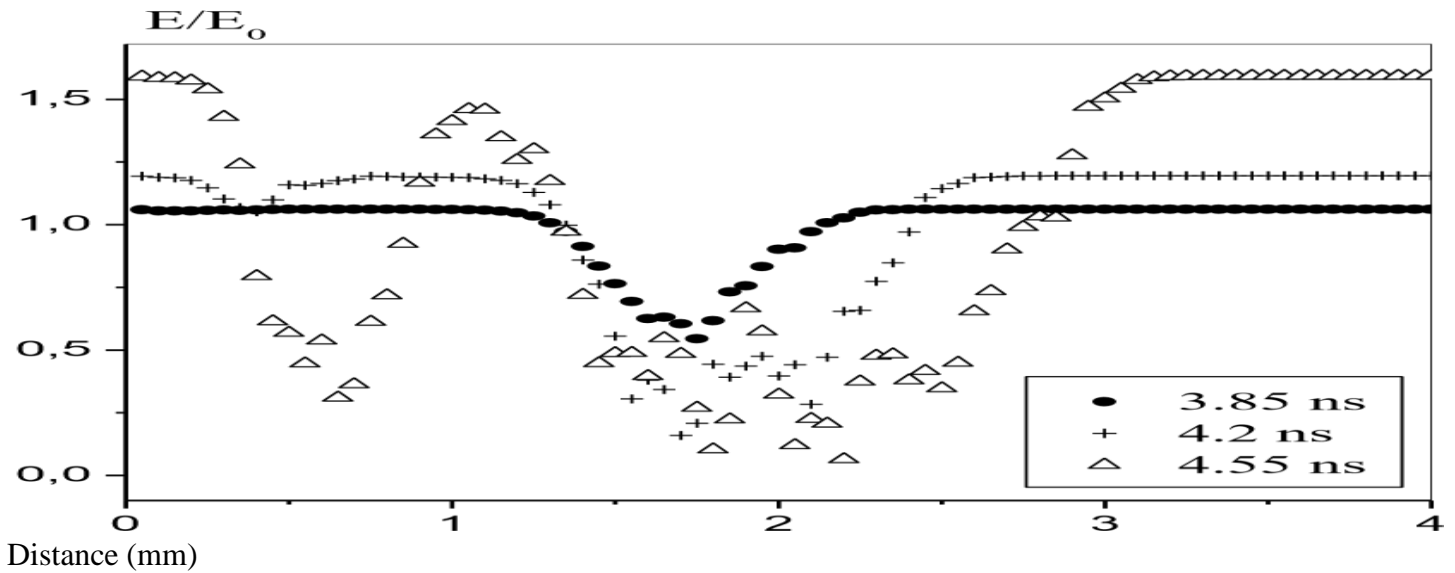


Fig. 16 Ratio of the local electric field to the applied field

The Monte Carlo method is applied to simulate the streamer discharge in SF_6 with the applied reduced electric field of 410 Td, the investigated gas density is $2.12 \times 10^{24} \text{ m}^{-3}$. The interval of the simulation must be less than the mean flight time; the electrons in the Monte Carlo simulation of the streamer discharge are followed at the same time intervals for to make calculations based on time and the electrons and ions, if exceeding a certain number, distort the electric field. In this study the mean flight times, $dt=0.35 \times 10^{-11} \text{ s}$ is chosen in the simulation, and the simulation interval is divided into equal domains with a length of $5 \times 10^{-3} \text{ cm}$. Near the cathode a number of electrons are injected with a low energies (0.1 eV), these electrons under the influence of the applied electric field move towards the anode. In areas of weak electric field, elastic collisions of electrons lower their energies, which slow them down in their movement towards the anode and cause attachments to the SF_6 molecules. For the strong enough electric fields the electrons are accelerated and inelastic collisions occur between the electrons and the SF_6 molecules. These inelastic collisions cause new electrons and positive ions of SF_6 , these charged particles form avalanches of electrons and zones of space charges which will change the value of the electric field. The local electric field due to the applied electric field added to the electric field caused by the space charge directs the propagation of the streamer. In front of the head of a streamer the electrons produced by the photoionization have an important role in the direction and propagation of the streamer discharge. The applied electric reinforced in the head of the initiation of the streamer by the electric field created by the space charge of the initials ionizations in the SF_6 produces the new ionizations which propagate the streamer. To regenerate avalanches in front and behind the first avalanche due to ionizations another process is necessary, this is photoionization. De-excitations of excited SF_6 molecules by the processes of collisions emit photons in front and behind the avalanches which cause the photoionization process. This new source of electrons and positive ions will increase the primary and secondary avalanches; this is the streamer discharge and propagates towards the anode and cathode. In the secondary avalanches the increase occurs on the axis of the main avalanche where the local field is important. The positive ions due to ionizations and photoionizations caused by secondary and primary avalanches will increase the electric field in front of and behind avalanches; this process allows regeneration and propagation of streamer discharge. From 3.85 ns after the application of the electric voltage the distortion of the electric field in

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the interval is very significant and important (Fig. 16). We notice that the local electric field is very large in front of, between and behind the avalanches which accelerates them. Figures 10-13 show the appearance of the second and third streamers which are due to photoionization and the local electric field. These processes are necessary in the development, regeneration and propagation of streamer discharge. The photoionization ahead of avalanches is very important and necessary because it explains the rapidity of the triggering of the electric discharge and the breakdown of the gap. In the simulation with the technique of Monte Carlo the calculated velocity of the propagation of the streamer discharge is 5.1×10^7 cm/s. They are a good agreement with the results investigations in the literature [28-29]. The faults in the high voltage systems and other problems are caused by the non-uniform electric field, the development and propagation of the electric discharge in such electric fields is necessary. For the simulation with the Monte Carlo method the corona discharge the cell size and the time step are important. The corona discharge is performed in a point-plane interval; with a fine mesh we calculate the electric field in the region where the variation is rapid. So the interval of the point-plane is divided in two subregions one next to the point electrode with a small size of the cells, and the other with a larger cell size is the rest of the interval. We apply the Monte Carlo technique to simulate the corona discharge; the advantage of using this method is that the transport parameters are not necessary. The simulation of the corona discharge is carried out for the negative polarity in the geometry of point to plane in SF₆ at 3 kV and the gas number density $N=2.12 \times 10^{24}$ m⁻³. A number of electrons are injected at the cathode at $t=0$ with 0.1 eV, the negative high voltage is applied to the point electrode and the plane electrode is grounded; the simulation is done in space and time. Through the process of ionization and photoionization, avalanches of electrons are formed as well as a positive space charge which will modify the electric field between the electrodes. Electrons with low energies caused by ionization of the SF₆ with electrons energies close to the ionization threshold, these low energy electrons can attach to SF₆ molecules. This phenomenon can cause a reduction of electrons and development and propagation of the avalanches. The positive space charge caused by the ionization of the molecules of SF₆ and the movement of electron avalanches towards the plane electrode enhances the local electric field at the both ends of the electron avalanche and weakens it in the center of this avalanche. In the area of the high electric field the ionization process causes a high number of positive ions, the electric field due to the positive space charge is higher than the applied field. All this induces a negative sign of the local electric field since the electric field of the space charge is higher than that of the applied field with an opposite direction. After the initialization of the electron avalanches at the point, the densities of electrons increase (Fig. 17). The decreasing of the local electric field induces the process of attachment which implies a decrease in the number of electrons. The process of attaching Electrons to SF₆ molecules causes a decrease in the value of the peaks of electron densities as they move towards the plane electrode (Fig.18).

Net (10^{10} cm⁻³) N⁺ (10^{12} cm⁻³)

1, 0

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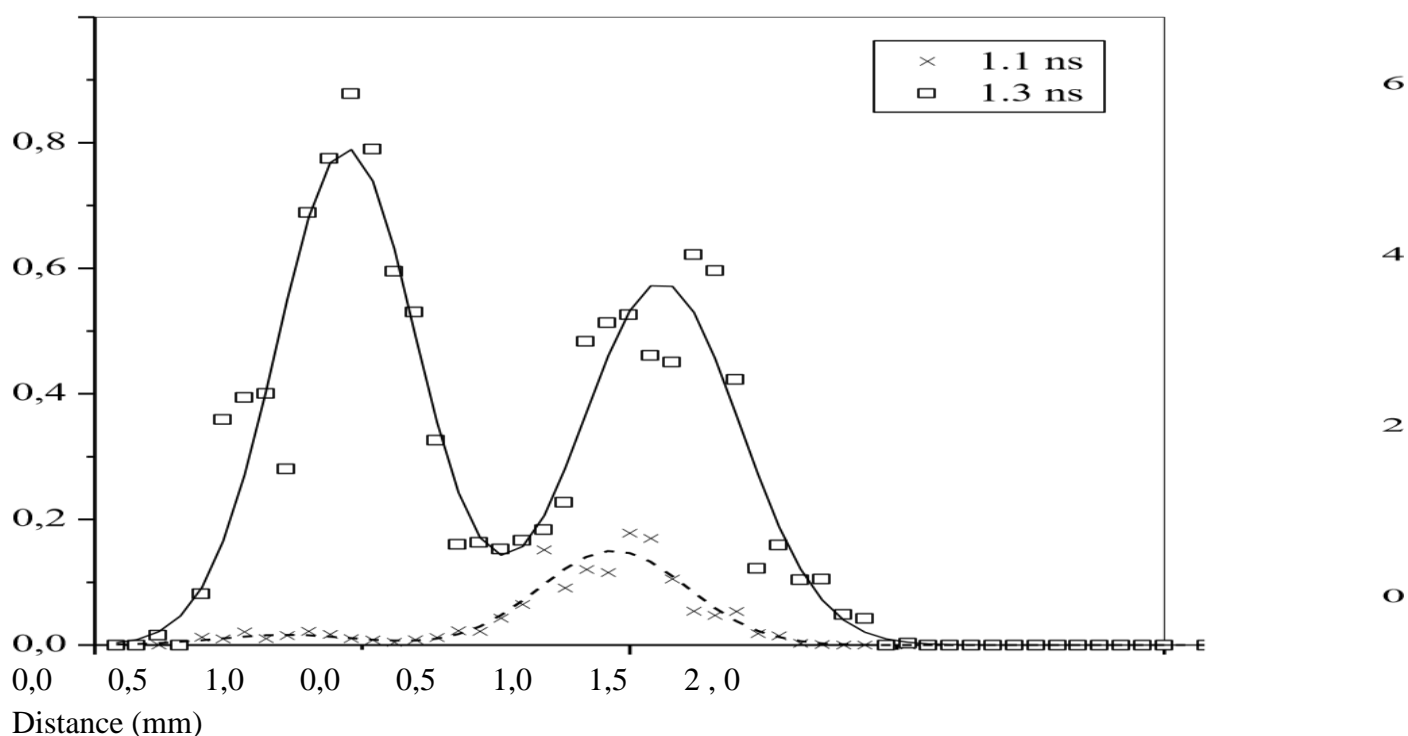
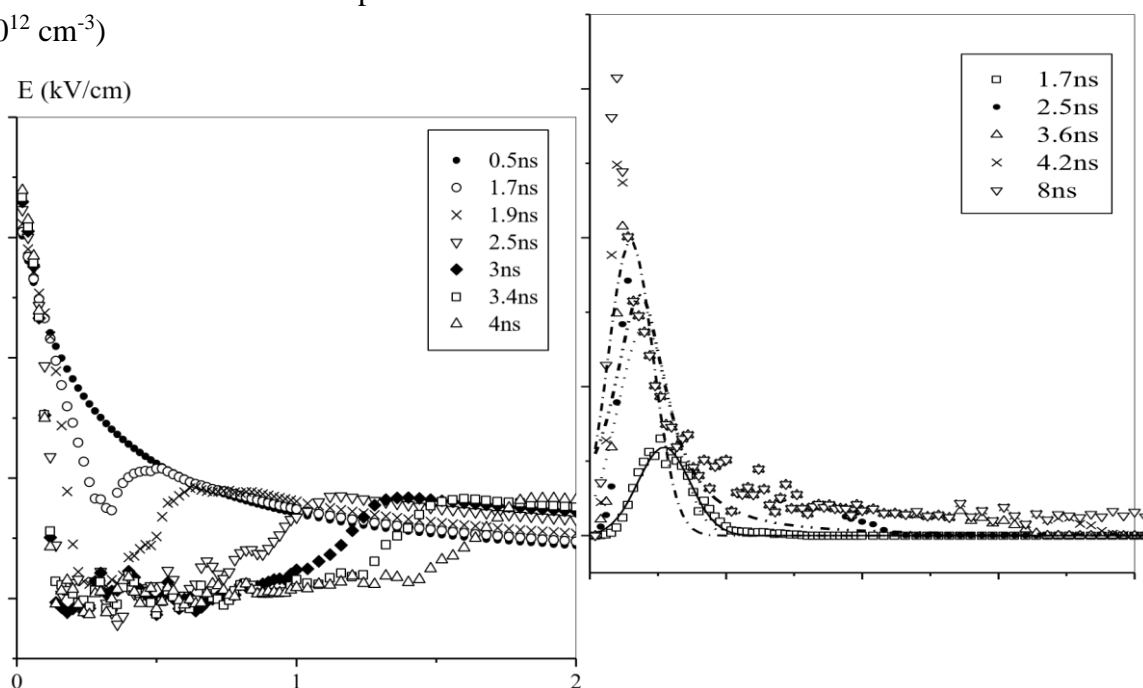


Fig. 17. Electron avalanches.Distance (mm)

Fig. 19. Evolution of the densities of positive ions.
40 Ne (10^{12} cm^{-3})



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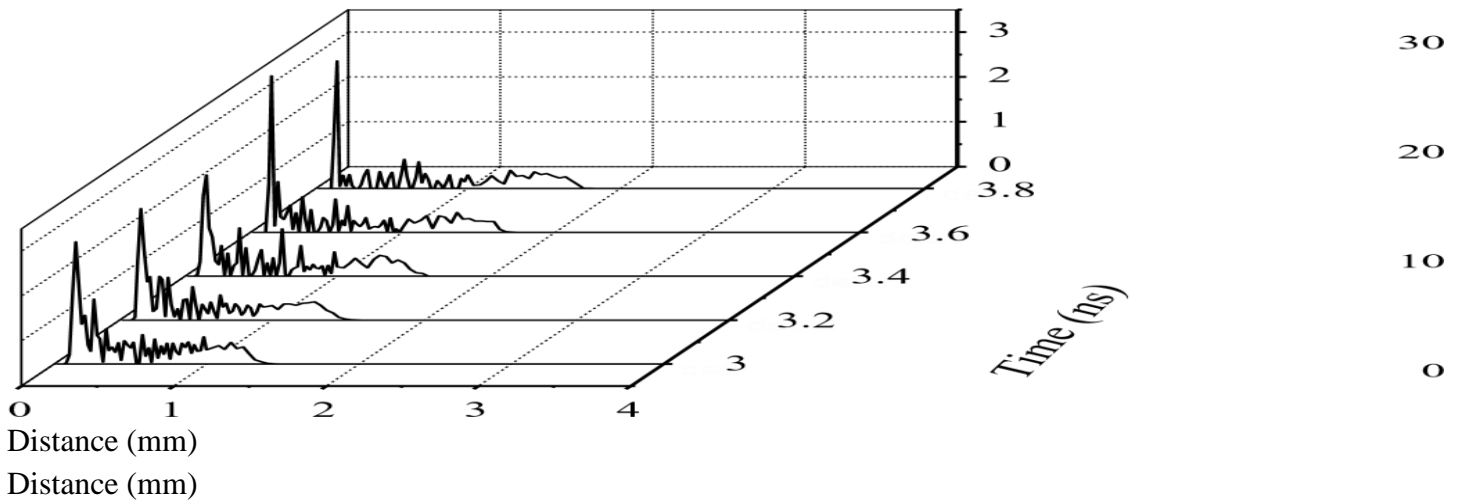


Fig. 20. Variation of the local electric field. Fig. 18. Electron avalanches.

The photoionization process creates electrons throughout space, those close to the plane electrode are in a weak electric field and through the attachment process will form negative ions, while those close to the point electrode will create other avalanches. The decrease in the local electric field moving towards the plane electrode will imply a decrease in the values of the peaks of the densities of the charged particles (Fig. 19). The generation of new corona discharge pulses is done by the electrons created near the point electrode by the photoionization process. Without this photoionization process there would be no initiation of new avalanches and the phenomenon will be extinguished due to lack of new electrons in the space where the local electric field is higher (Fig. 20). Successive new avalanches will be created near the tip electrode and will move towards the flat electrode while growing, up to a maximum then begin to decrease in the regions of weak local electric field. The velocities of the propagation of electron avalanches calculate using the Monte Carlo method it is around of 3×10^7 cm/s to 4×10^7 cm/s. These calculated velocities are in good agreement with the experimental results referred to in [30-34] The result obtained with the Monte Carlo method show with this technique we can simulated the electron transport parameters and the initiation and propagation of the streamer and corona discharges.

4. Conclusion

The swarm parameters in gases are necessary for the simulation of the process that uses discharges and plasma in technological applications. We have used the Monte Carlo kinetic method to calculate the electron transport parameters in the SF₆ and to track the charged particles in space and time. Several processes with the SF₆ molecules produce electrons and ions, the charged particles start other avalanches and create space charges which cause a change in the local electric field. All those imply the phenomena of initiation and propagation of streamer and corona discharges. By Monte Carlo simulation method we have studied the streamer and corona discharges formation and propagation in SF₆. The change in the local electric field due to the positive space charge has been studied. The distributions of the charged particles as a function of time and distance between electrodes are calculated. The photoionization process it is necessary and important in the propagation and regeneration of avalanches in the streamer and corona discharges. The simulation with the Monte Carlo technique gives us detailed results of the structures and propagation of avalanches one after the other.

References

Original Article

- J.Y. Kim, I. Kaganovich and H.C. Lee, Review of the gas breakdown physics and nanomaterial-based ionization gas sensors and their applications, *Plasma Sources Sci. Technol.* 31 (2022) 033001.
- J. Nishimura, K. Takahashi, K. Takaki, S. Koide, M. Suga, T. Orikasa, Y. Teramoto, T. Uchino, Removal of ethylene and by-products using dielectric barrier discharge with Ag nanoparticle-loaded zeolite for keeping freshness of fruits and vegetables, *Trans. Mat. Res. Soc. Japan.* 41 (2016) 41-45. [3]. R.M.A. Velásquez, Insulation failure caused by special pollution around industrial environments, *Engineering Failure Analysis* 102 (2019) 123–135.
- Y. Si, Y. Yang, M. Martel, L. Zhang, S. Kirychuk, B. Predicala, H. Guo, Characterization of electrical current and liquid droplets deposition area in a capillary electrospray, *Results in Engineering* 9 (2021) 100206.
- C. Lee, J. Kim, J. Yoon, Inactivation of MS2 bacteriophage by streamer corona discharge in water, *Chemosphere* 82 (2011) 1135–1140. [6]. A. Božovic, K. Tomašević, N. Benbettaieb, F. Debeaufort, Influence of surface corona discharge process on functional and antioxidant properties of bio-Active coating applied onto PLA films, *Antioxidants* 12 (2023) 10.3390.
- L. Zhao, L. Xie, C. Liu, L. Gao, J. Qu, H. Zhang,
- Y. Liu, Corona current and audible noise characteristics of HVDC transmission lines and their relationship at high-altitude, *IET Gener. Trans. Distrib.* 1 (2023) 10.1049/gtd2.12832.
- S. Wilczek, J. Schulze, R. P. Brinkmann, Z. Donkó, J. Trieschmann, T. Mussenbrock, Electron dynamics in low pressure capacitively coupled radio frequency discharges, *J. Appl. Phys.* 127 (2020)
- W. Yang, X. Meng, Q. Zhou, Z. Dong, Boltzmann equation studies on electron swarm parameters in Townsend breakdown of copper vapor plasma using independently assessed electron-collision cross sections, *AIP Advances.* 9 (2019) 10.1063/1.5048982. [10]. A. P. Jovanovic, M. N. Stankov, V. Lj. Markovic, S. N. Stamenkovic, Simulation of the statistical and formative time delay of Townsend mechanism-governed breakdown in argon at low pressure, *Contrib. Plasma Phys.* (2023) 10.1002/ctpp.202200161.
- M. Zhang, H. Zhang, Prediction of the breakdown voltage and breakdown area of gas switches based on ionization integral, *AIP Advances.* 13 (2023) 10.1063/5.0121607.
- J. Paz-Martín, A. Schüller, A. Bourgouin, D. M.
- González-Castaño, N. Gómez-Fernández, J. PardoMontero, F. Gómez, Numerical modeling of airvented parallel plate ionization chambers for ultrahigh dose rate applications, *Physica Medica* 103 (2022) 147–156.
- A. Tentori, A. Colaitis, D. Batani, 3D MonteCarlo model to study the transport of hot electrons in the context of inertial confinement fusion. Part II, *Matter and Radiation at Extremes.* 7 (2022) 10.1063/5.0103632.

Original Article

- L. N. Mai, T. H. Vu, T. X. Dinh, H. D. Vu, C. D. Tran, V. T. Dau, H. K. Ngo, Numerical study of electrohydrodynamic atomization considering liquid wetting and corona discharge effects, *Phys. Fluids*. 35 (2023) 10.1063/5.
- X. Zhang, J. Wang, F. Wang, W. Fan, Particle simulation of positive streamer discharges on surface of DC transmission conductors with coating materials, *IEEE Trans. Plasma Science*. 50 (2022) 3751-3759.
- V. F. Tarasenko, E. Kh. Bakshta, E. A. Sosnina, A. G. Burachenkoa, V. A. Panarina, V. S. Skakuna, Characteristics of a pulse-periodic corona discharge in atmospheric Air, *Plasma Phys. Rep.* 44 (2018) 520532.
- S. H. Nam, H. Rahaman, H. Heo, S. S. Park, J. W. Shin, J. H. So, W. Jang, Empirical analysis of high pressure SF₆ gas breakdown strength in a spark gap switch, *IEEE Trans. Dielect. Electr. Ins.* 16 (2009) 11061110.
- M. Radmilović-Radjenović, B. Radjenović, Theoretical studies of the electrical discharge characteristics of sulfur hexafluoride, *J Electr Eng Technol.* 12 (2017) 288-294.
- Y. An, K. Yin, T. Huang, Y. Hu, C. Ma, M. Yang, B. An, D. Chen, Study on the insulation performance of SF₆ gas under different environmental factors, *Frontiers in Phys.* (2022) 820036. [20]. R. Zhang, L. Wang, J. Liu, Z. Lian, Numerical simulation of breakdown properties and streamer development processes in SF₆/CO₂ mixed gas, *AIP Advances*. 12 (2022) 015003.
- C. Ding, Q. Ding, Z. Wang, Y. Zhou, C. Chen, Comparison of algorithms for predicting plasma physical parameters of SF₆-Cu mixtures at local thermodynamic equilibrium state via machine learning, *AIP Advances*. 11 (2021) 115102. [22]. P. Priyadarshi, N. Neophytou, Computationally efficient Monte Carlo electron transport algorithm for nanostructured thermoelectric material configurations, *J. Appl. Phys.* 133 (2023) 054301. [23]. A. Settaouti, Monte Carlo simulation of electron swarm parameters in O₂, *Eur. Phys. J. Appl. Phys.* 37 (2007) 335-341.
- A. Settaouti, Monte Carlo simulation of avalanche formation and streamer discharge, *Electr Eng* 92 (2010) 35-42.
- A. Settaouti, Numerical simulation of the formation and propagation of streamer, *International Journal of Modern Physics C*. 18 (2007) 957-971. [26]. A. Settaouti, Characterization of point-plane corona discharge in oxygen with Monte Carlo method, *Physics Journal*. 4 (2018) 1-8.
- A. Settaouti, Numerical simulation of corona discharge in N₂, *J. Electr.* 65 (2007), 625-630. [28]. A. Komuro, R. Ono, T. Oda, Effects of pulse voltage rise rate on velocity, diameter and radical production of an atmospheric-pressure streamer discharge, *Plasma Sources Sci. Technol.* 22 (2013) 045002.
- B. Qi, D. Yu, Numerical simulation of the negative streamer propagation initiated by free metallic particle in N₂/O₂ mixtures under non-uniform field, *Processes*. 12 (2024) 1554.