CALCULATION OF ELECTRON SWARM PARAMETERS OF c-C_4F_8/N_2 MIXTURES USING AN IMPROVED MONTE CARLO COLLISION SIMULATION METHOD

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ABSTRACT

This paper analyses the insulation characteristics of c-C_4F_8/N_2 gas mixtures using the improved Monte Carlo method with the null-collision technique and studies the possibility of applying that in the gas insulation of power equipment. The density-normalized effective ionization coefficient $(\alpha-\eta)/N$ for c-C_4F_8/N_2 gas mixtures has been calculated using a sample of a pulsed Townsend discharge. The overall density-reduced electric field strength E/N could be varied between 160 and 480 Td (1Td = 10^{-21} V m^2), while the c-C_4F_8 content in the gas mixtures is varied over the range 0–100%. From the variation curve of $(\alpha-\eta)/N$ with the c-C_4F_8 mixture ratio k, the limiting field $(E/N)_{\lim}$ of the gas mixture at different gas contents is determined. The required gas pressure ratios comparable to the insulation property of SF_6 and the global warming potential (GWP) at this gas pressure were also investigated. It is found that the dielectric strength of c-C4F8/N_2 mixtures is less than that of the SF_6/N_2 gas mixture at k below 60%, and is larger at k above 60%, and the GWP of the former is significantly lower than that of the latter.

1. INTRODUCTION

Recently, the high global warming potential (GWP) of SF6 gas has once more stimulated active studies aimed at searching for a substitute gas with lower environmental impact[1] as the insulating medium. Perfluorocyclobutane (c-C_4F_8) is a processing gas employed in plasma etching, with possible utilization as a gaseous dielectric especially in gas mixtures[2] and with potential for lowering global warming gas emissions[3]. The GWP of c-C_4F_8 is 8700[2], only about 36% of that of SF_6. As a gas insulator c-C_4F_8 has no toxicity ozone destructing potential[1], excellent thermal stability[2,4] and high dielectric strength. But c-C_4F_8 has a low boiling point, so an ordinary gas such as N_2, CO_2, air or CF_4 constituting the greater portion of a mixture, might increase the boiling point of the mixture[1]. So we think that c-C_4F_8 is a promising component gas of a mixture as an insulation candidate of substitute for SF_6 gas.

Binary mixtures of c-C_4F_8 with N_2 have been suggested as possible replacements of SF_6 in high voltage insulation applications[5,6]. So studies on electron swarm coefficients and dielectric strength on the c-C_4F_8 and N_2 gas mixtures are essential. However, theoretical studies have been mostly conducted in pure N_2 or pure c-C_4F_8 discharges, studies in gas mixtures being rare. So in this paper, an improved Monte Carlo simulation method is used to calculate the effective ionization coefficients for the c-C_4F_8/N_2 gas mixtures. The limiting fields, the value of $(E/N)_{\lim}$ at which $(\alpha-\eta)/N=0$, are obtained by the $(\alpha-\eta)/N$ curve and then compared with that of SF_6/N_2 gas mixtures. The results show that the limiting fields of c-C_4F_8/N_2 gas mixtures are comparable with the SF_6/N_2 gas mixtures. The simulation results show that the c-C_4F_8/N_2 gas mixtures are a desirable synergistic mixture which is consistent with the experimental data available in the paper.

2. THE SIMULATION METHOD

Itoh and Musha[7] apply the Monte Carlo method to electron transport at first. The null-collision technique, introduced by Skullerud[8], is widely used. In this work, we use the improved Monte Carlo method with the null-collision technique to simulate the electron swarm of c-C4F8/N2 mixtures in uniform fields. The gas number density is N = 3.29×10^{22} m^{-3} in the pressure of 1 Torr at 20℃. It is assumed that the electron density is sufficiently small, so the Coulomb interactions between the particles as well as shielding of the field are negligible[9]. The procedure of the Monte Carlo method is described in[7–12]. Hence, a brief overview of this method is given. The uniform electric field E is antiparallel to the z-axis. At time t

= 0, n_0 initial electrons are released from the origin of the coordinate system with a constant energy of 1.0 eV.

At a given electron energy ε, the total collision cross section (CS) of the mixture $Q_t(\varepsilon)$ is given as

$$Q_t(\varepsilon) = kQ_{c-C_4F_8}(\varepsilon) + (1-k)Q_{N_2}(\varepsilon) \quad (1)$$

where k is the fractional c-C_4F_8 content in the mixture and $Q_{c-C_4F_8}(\varepsilon)$ and $Q_{N_2}(\varepsilon)$ are the total collision CSs of c-C_4F_8 and N_2, respectively.

In this method the maximum collision frequency $\nu_{\max}$ of the gas mixture is defined for the range of electron energy 0–100eV, using the formula $V(\varepsilon) = \sqrt{2\varepsilon e/m}$ and $\nu = N|V(\varepsilon)|Q_t(\varepsilon)$, the collision frequency, ν can be calculated out corresponding to ε; so we may find the maximum collision frequency $\nu_{\max}$, where ε is the electron energy, e is the electronic charge, m is the electronic charge mass, N is the gas number density and $V(\varepsilon)$ is the electron velocity. If an electron collides, it will lose energy. We find that the electron energy generally does not exceed 50eV in the simulation process in the predetermined termination time t. It's supposed that for each electron not only real collisions but also null collisions occurs. For the CS of a null collision $Q_{null}(\varepsilon)$ is as follows:

$$\nu_{\max} = N\{|V(\varepsilon)|[Q_{null}(\varepsilon) + Q_t(\varepsilon)]\} \quad (2)$$

$$\nu_{real} = N|V(\varepsilon)|Q_t(\varepsilon) \quad (3)$$

$$P_{real} = \nu_{real}/\nu_{\max} \quad (4)$$

$$dt = -(\ln R_1/\nu_{\max}) \quad (5)$$

where $R_1(R_m, m = 1,2,3,\cdots)$ are the random numbers uniformly distributed between 0 and 1, ν_{real} is the collision frequency of a real collision, P_{real} is the real collision probability and dt is the actual flight time. If $P_{real} > R_2$ the collision is real, otherwise the collision is null and we proceed to the next collision without any change in electron energy and direction [13]. In a collision event, colliding with which gas molecule type is determined by

$$P_1 = (1-k)\nu_{N_2}/\nu_{mix} \quad (6)$$

$$P_2 = (k\nu_{c-C_4F_8}/\nu_{mix} \quad (7)$$

$$\nu_{mix} = (1-k)\nu_{N_2} + k\nu_{c-C_4F_8} \quad (8)$$

$$P_1 + P_2 = 1 \quad (9)$$

where ν_{N_2} and $\nu_{c-C_4F_8}$ are the collision frequencies for N_2 and c-C_4F_8 in the process of collision, respectively. If $R_2 \le P_1$, the electron collides with the N_2 gas molecule, or else if $R_2 \le P_1 + P_2$, the electron collides with the c-C_4F_8 gas molecule. The nature of collisions for N_2 and c-C_4F_8 is determined by $Q_{(j,1)}(\varepsilon)/Q_{N_2}(\varepsilon)$ and $Q_{(j,2)}(\varepsilon)/Q_{c-C_4F_8}(\varepsilon)$ where $Q_{(j,1)}(\varepsilon)$ and $Q_{(j,2)}(\varepsilon)$ are the CSs of the jth collision process for N_2 and c-C_4F_8, respectively. Isotropic scattering in the system is assumed. After a collision event, a new direction for the electron is decided by the scattering angle θ, $\theta = \cos^{-1}(1-2R_3)$, and the azimuthal angle φ, $\phi = 2\pi R_4$. After an elastic collision, the electron energy change is decided by

$$\varepsilon_l = \varepsilon_0[1 - \frac{2m_e}{M_i}(1-\cos\theta)] \quad (10)$$

where ε_0 is the electron energy before the collision and m_e and M_i (i = 1, 2) are the electron and c-C_4F_8 and N_2 molecule mass, respectively. After an inelastic collision (vibration, excitation, dissociation, ionization and attachment collisions), the electron energy change is retained by $\varepsilon_l = \varepsilon_0 - \Delta\varepsilon_j$, where $\Delta\varepsilon_j$ is the threshold energy for each inelastic collision process.

For the ionization collision, after subtracting the threshold energy $\Delta\varepsilon_{ion}$, the energy of the primary and secondary electrons of c-C_4F_8 and N_2 is determined by $(1-R_5):R_5$, respectively. If the electron is attached (electronegative gases only) it stops moving. The simulation stopping criterion is a predetermined termination time t; at this time information of all new electrons and previous electrons is stored. We use C language to program the present simulation code.

Although every electron in the swarm moves at its own velocity, the electron swarm as a whole moves with the drift velocity V_e parallel to the field direction[14]. The drift velocity V_e is defined as the average velocity of all the electrons in the swarm. The drift velocity V_e is calculated by the method of Dincer[10].

$$V_e = \frac{\bar{z}}{t} \quad (11)$$

where $\bar{z}$ is the average distance traveled in the field direction at the predetermined termination time t.

The ionization α and attachment η coefficients are calculated by the method of Dincer[10] and Raju[13].

$$\alpha = \frac{\ln[(n/n_0)+1]}{\bar{z}} \quad (12)$$

where n is the number of new electrons produce in the electron swarm with ionization.

$$\eta = \frac{n^-}{n^+}\alpha \quad (13)$$

where n^+ and n^- are the numbers of positive and negative ions produced in the electron swarm.

3. CROSS SECTIONS

For this simulation experiment by Monte Carlo method, we select the momentum transfer CS from L.G. Christophorou[2], vibrational excitation CS with a threshold energy of 0.15 eV and electronic excitation CS with a threshold energy of 8 eV from Skullerud[8] and ionization CS with a threshold energy of 14 eV, neutral dissociation CS with a threshold energy of 10 eV and attachment CS from [2] as the initial CSs set. In order to obtain agreement with the measured electron swarm parameters, we make some modifications for electron collision CSs of c-C_4F_8 according to the following three steps. (i) The attachment and electronic excitation CSs are modified to make $(\alpha-\eta)/N$ agreement with the experimental values. (ii) The momentum transfer CS is now modified to make the V_e agreement with the experimental values. (iii) The above two steps are repeated until electron swarm parameters agree with the experimental values. At last, we multiplied the attachment CS for the formation of c-C_4F_8 by 0.01 same with [3] and for $1 \leq \varepsilon < 4$ eV by 0.1; the electronic excitation CS for $8 < \varepsilon \leq 14$ eV by 0.5 and for $14 < \varepsilon \leq 100$ eV by 0.2. The final electron collision CSs set of c-C_4F_8 is shown in Fig.1. The CS of N_2 is taken from Phelps and Pitchford [15,16].

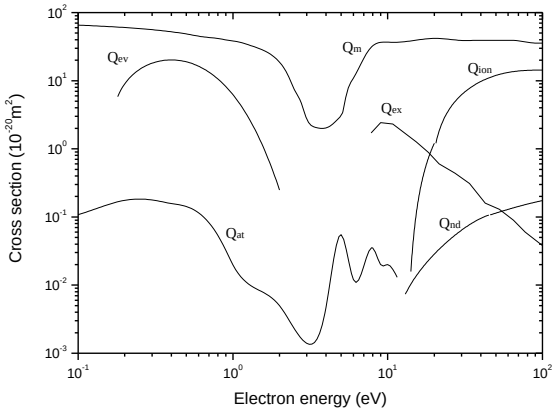

Fig.1 *Final CS for c-C_4F_8: Q_m elastic momentum transfer; Q_{ev} vibrational excitation; Q_{ex} electronic excitation; Q_{ion} ionization; Q_{nd} neutral dissociation; Q_{at} t electron attachment.*

4. SIMULATION RESULT AND DISSCUTION

The effective ionization coefficient of c-C4F8 and N_2 gas mixtures are obtained by simulation as a function of E/N at a constant mixing ratio as shown in figure 2. The results indicate that the effective ionization coefficient $(\alpha-\eta)/N$ increases with the increase in E/N, while $(\alpha-\eta)/N$ decreases with the c-C4F8 gas content (k), and this reduction in the effective ionization coefficients becomes relatively larger as k increases.

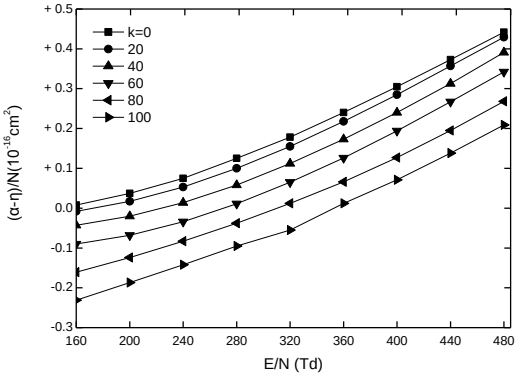

Fig.2 *Effective ionization coefficient $(\alpha-\eta)/N$ in c-C_4F_8 and N_2 mixtures as a function of E/N at different c-C4F8 gas mixture ratio k*

The value of $(E/N)_{\lim}$ is deduced from the effective ionization coefficient in figure 2, and given in figure 3 as a function of k for c-C4F8/N_2 mixtures. The E_s/N value measured by James et al[17]. Here, E_s is the dielectric breakdown strength. Despite a difference in gas number density, a comparison shows good agreement between the present $(E/N)_{\lim}$ values and the measured E_s/N ones. Because SF_6/N_2 are now widely studied as the most plausible SF_6 gas mixture, their experimental data[18] are also given in figure 3 for comparison. It is obvious that the dielectric strength of c-C4F8/N_2 mixtures is less than that of the SF_6/N_2 gas mixture at k below 60%, and is larger at k above 60%.

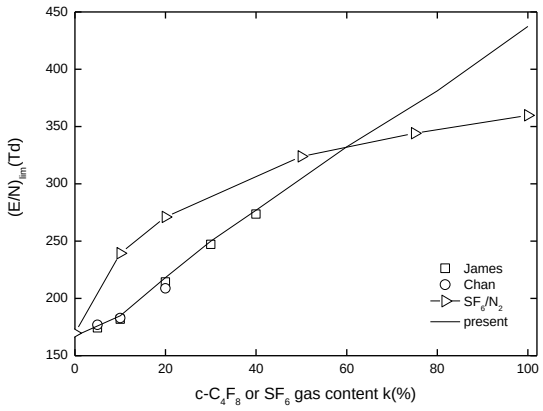

Fig.3 *The limiting fields $(E/N)_{\lim}$ as a function of c-C_4F_8 or SF_6 gas content k (experimental data: James et al, Chan et al, SF_6/N_2 and c-C_4F_8/N_2).*

Under the conditions that presumed the insulation

characteristics were proportional to gas pressure, the required gas pressure ratios comparable with the insulation property of SF_6 and GWP at this gas pressure were also investigated, and are given in figures 4 and 5. It is obvious that the GWP of c-C4F8/N_2 is greatly reduced for the same SF_6 or c-C_4F_8 gas mixture ratio, while the pressure ratio required for both gas mixtures is almost the same. For example, the pressure of the 20% c-C4F8/N_2 gas ratio was 1.6528 and the GWP ratio was 0.0728, one-tenth and one-third of that of pure SF_6 and SF_6/N_2 respectively.

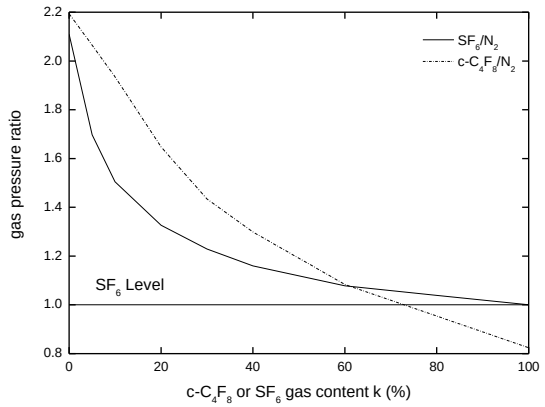

Fig.4 *Required gas pressure ratio compared with insulation property of SF_6.*

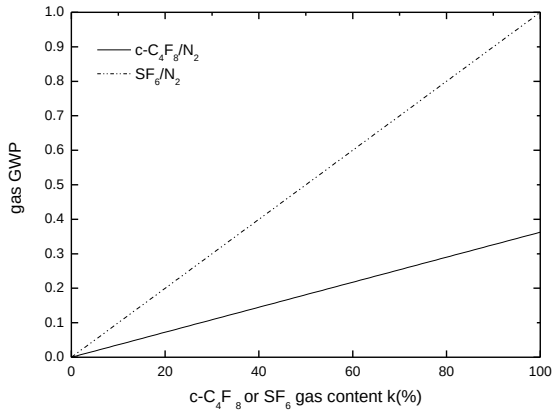

Fig.5 *GWP of gas mixtures relative to SF_6.*

5. CONCLUSION

The electron effective ionization coefficient and the limiting field strength for c-C4F8/N2 mixtures have been calculated for a range of E/N from 160 to 480 Td by the improved Monte Carlo method. It can be seen that c-C4F8/N2 gas mixtures are desirable synergistic mixtures whose insulation strength can be comparable to that of SF6/N2 gas mixtures, but the GWP is greatly reduced. From environmental, physical and electrical aspects, we suggest that c-C4F8/N2 gas mixtures are possible substitutes for SF6 and SF6/N2 gas mixtures. There are still many theoretical and experimental researches that need to be finished. We are prepared for the experimental set-up, and will measure the AC breakdown voltage of c-C_4F_8/N_2 gas mixtures by experiments in a uniform field to validate the simulation results in future works.

6. REFERENCES

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