Net Emission Coefficient of Nitrogen-PTFE Gas Mixture in Thermal and Chemical Equilibrium

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The net emission coefficient (NEC) of pure nitrogen gas and its mixture with PTFE vapour in plasma state is calculated over the pressure range of 1 to 100 bar and temperature range of 300 to 35,000 K. 26 species are included in the NEC calculation for N_2-PTFE mixture. Results are compared with existing data to assess the applicability of the method.

Keywords: NEC, nitrogen, PTFE, radiation

1 INTRODUCTION

Radiation is a principal energy loss mechanism at the centre of high current switching arcs (>1000 A). The modelling of radiation transfer is often based on the concept of net emission coefficient (NEC) [1, 2] although more accurate but computing intensive methods exist, such as the Partial Characteristics Method [3] and the Discrete Coordinate Method [4]. In the present work the NEC of pure nitrogen and its mixture with PTFE vapour in thermal and chemical equilibrium plasma state is calculated in order to provide baseline information for the development of SF_6 free switching technology.

2 CALCULATION METHOD

2.1 EQUILIBRIUM COMPOSITION

A total of 26 species are taken into account in the calculation of the plasma composition, based on the method of Godin and Trepanier [5] which is based on the minimisation of a chemical potential. 4 species are set as the chemical bases in consideration of the number of chemical elements present in the plasma and the charge (N, C, F, and charge). Therefore, the rest 22 species are set as chemical species and mass action law is applied. The principles of conservation of atomic nucleus, electrical neutrality and ideal gas law are used for the closed system of plasma. A total of 26 equations are obtained, which include two equations for conservation of nuclei (ratio of C:F in PTFE + N:F between PTFE and N_2), one equation for charge neutrality, one from the ideal gas law and another 22 equations describing the mass action law for the 22 chemical species. These equations are solved using the Newton-Raphson method to obtain the number density of all 26 species. Logarithm was taken on both sides of the chemical species equations, which results in 22 linear equations and greatly simplifies the calculation. The linear equations are then substituted in the base equations to reduce the number of unknowns to only 4. This gives a smaller size of the Jacob matrix in the solution procedure using the Newton-Raphson Method, which substantially promotes the convergence of the calculation.

The Fermi and Griem criteria are used in the determination of the internal partition functions (IPFs) based on the work of Drellishak [6] and D'Angelo [7]. The IPFs of atom and its ions are calculated using the electronic energy levels and degeneracies taken from NIST database [12]. The IPFs of molecules are calculated by the method in [9].

The composition for N_2-PTFE mixture is shown in Fig.1. Details of the composition at low temperature is shown in Fig.2. Molecules (N_2, C_2F_4, and CF_3) are the dominant species when the temperature is lower than 4,000 K.

Due to rapid dissociation of C_2F_4, CF_3 is generated at 1,200 K and reaches its peak value of $4.5\times10^{23}/m^3$ at 3,500 K. Atomic fluorine becomes the dominant species at 3,900 K and remains its dominance up to 16,000 K before electrons take over as the

most abundant species due to ionisation of atomic fluorine.

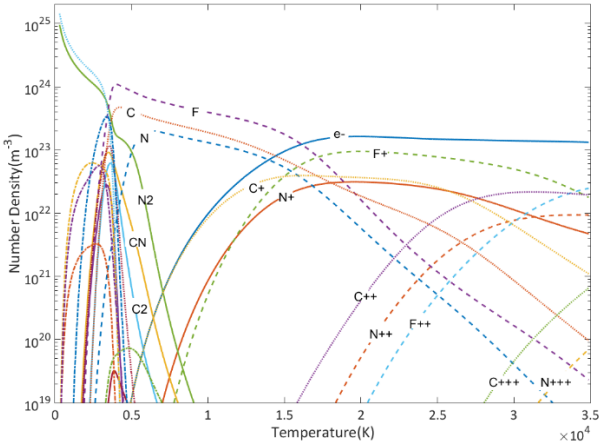

Fig. 1: Chemical equilibrium composition of 40% N2 – 60% PTFE mixture (volume) gas plasma at 1 bar. See Fig.2 for details over 300 K to 5000 K

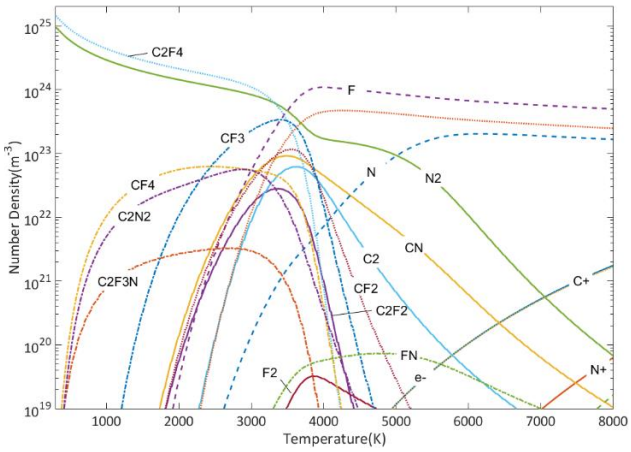

Fig. 2: Chemical equilibrium composition of 40% N_2 – 60% PTFE mixture gas plasma at 1 bar at low temperature

2.2 TOTAL ABSORTPION COEFFICIENT

In order to determine the NEC of the N_2-PTFE mixture, information on the total emission and absorption spectra is necessary.

a. Atomic continuum

For atomic continuum radiation, three important phenomena need to be taken into account: radiative attachment, radiative recombination and Bremsstrahlung. Radiative attachment is due to an atom capturing an electron, forming a negative ion and emitting a photon. The result in [8] appears to show smaller photoionization cross section for CN^-, C_3N^- and C_5N^- in comparison with other ions. It would appear that radiative electron attachment is negligible compared to neutral particle induced attachment. Radiative recombination makes the most contribution to the continuum radiation. The calculation makes use of the Scaled Thomas-Fermi potential [10]. The latest energy levels from NIST [11] and the work of Kurucz [12] are used. The Bremsstrahlung coefficient, known as the Gaunt factor [13], is used to correct the hydrogen-like approximation. The coefficient is calculated based on the method in [13].

b. Atomic lines

The total number of atomic lines considered in the calculation is 32644. The data of atomic spectral lines is obtained from NIST [11] with the spectral completed by the database from Kurucz [12]. The absorption oscillator strength is obtained from NIST database [11]. Stark broadening operates in most of the atomic lines [1]. In addition, both Doppler broadening and Van der Waals broadening are taken into account. The calculation of radiation due to electron transaction between different energy levels is described in [1].

2.3 NET EMISSION COEFFICIENT

The NEC is related to the spectral absorptivity K' by Kirchhoff's Law. It is obtained by

$$\varepsilon_N = \int B_v K' G_1(K'(v, \mathrm{T}, \mathrm{P})\mathrm{R})\, dv \qquad (1)$$

where B_v is the Planck function, R the thermal radius, v the frequency, T the temperature and P the pressure. G_1 is the geometry function which can be expressed as

$$G_1 = \int_0^{\pi/2} sin\theta \exp(-K' R/sin\theta)\, d\theta \qquad (2)$$

where θ is polar coordinate. In performing the summation of the absorptivity for all lines and continuum radiation, those lines with absorption oscillator strength less than 10^{-6} are omitted. In order to accurately represent the photon-absorption edges, absorption edges of frequency v_e and $0.999\, v_e$ are chosen as the integration points.

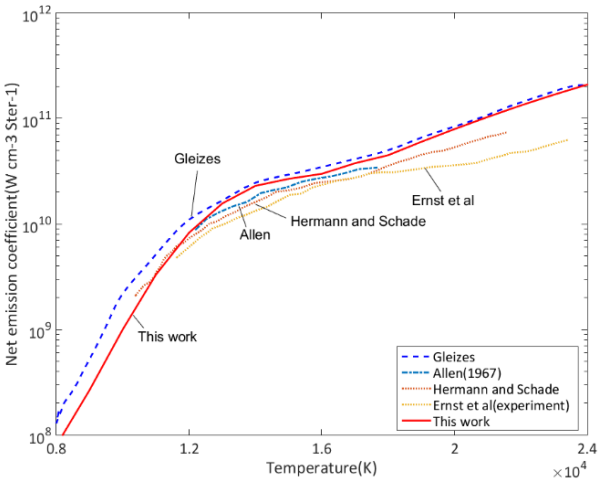

Fig. 3: Calculated NEC of pure nitrogen gas plasma comparing with existing results at 1bar

3 RESULTS AND DISCUSSION

Firstly, the results of NEC of pure Nitrogen are presented. Fig.3 shows available experimental and theoretical results on NEC with a zero plasma radius at 1 bar [14,15,16,17]. For a zero plasma radius (R=0), by definition self-absorption is not accounted for in the calculation. Results from the present work is close to those of Gleizes [14] for T > 13,000 K with a maximum percentage difference of 13.1%. The discrepancy of up to 29.5% below 13,000 K could be due to the difference in the atomic data used in [14] and in the present work where most up to date data are used. Fair agreement with the results of Allen [14] and Hermann [15] is achieved. Results of Ernst et al [16] were obtained from experiment. An increasing discrepancy is observed starting at 17,000 K, for which reasons are not yet clear.

Fig.4 shows the NEC for 40% nitrogen – 60% PTFE mixture with different plasma column radii. As the NEC is quite low at low temperature, results presented here are for temperature higher than 8,000 K. Initially the NEC increases rapidly with temperature. The rate of increases slows down when the temperature reaches 14,000 K. It is interesting to note that this pattern of rate of change of the NEC seems to be closely linked to the total number density of the ions. The rate of change of the NEC becomes higher again when the temperature exceeds 18,000 K, due to the increase in the population of the ions.

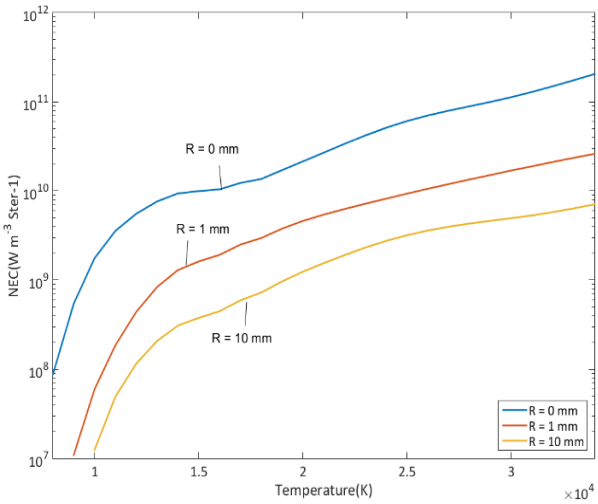

Fig. 4: NEC of 40% N_2 – 60% PTFE gas plasma with different R at 1bar

In the gas mixture calculation, two cases with 40% nitrogen - 60% PTFE (Case 1), and 80% nitrogen – 20% PTFE (Case 2) were selected as the initial composition. Fig.5 shows the NEC of r=0 with different compositions. The maximum difference in the NEC between the two cases below 15,000 K is about 30%. The difference increases again when the temperature is higher than 22,000 K. The NEC of Case 2 is 50% higher than that of the Case 1 at 34,000 K. This indicates that the influence of PTFE on the NEC can be significant, especially at high temperature (T > 22,000 K).

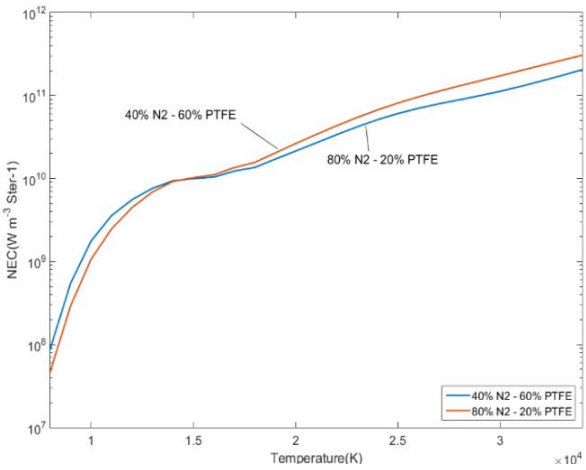

Fig. 5: Comparison between different compositions of N_2 – PTFE mixture gas plasma at 1 bar

Fig.6 presents the comparison of NEC between high pressure (100 bar) and low pressure (1 bar). Results indicate that the value of NEC can be significantly affected by

the gas pressure, but not in a linear relationship.

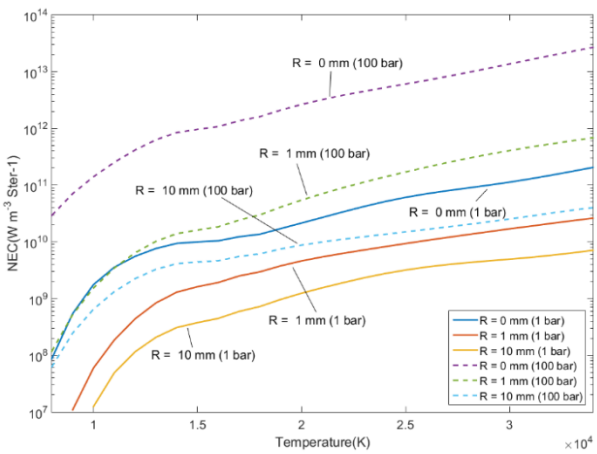

Fig. 6: Comparison of high pressure NEC 40% N_2 – 60% PTFE

4 CONCLUSION

The NEC of N_2-PTFE mixture has been calculated in the pressure range of 1 to 100 bar and initial volume concentration range of 0 to 100% of PTFE. Results indicate that the presence of PTFE vapour can substantially affect the NEC of switching arcs operating with nitrogen as the background gas. The difference of NEC values between different gas compositions can be as much as 30% - 50%. Pressure also affects the NEC significantly.

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