Boltzmann Equation Analysis and Monte Carlo Simulation of Electron Transport in N_2-O_2 streamer discharge

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We have calculated data for electron transport in mixtures of molecular nitrogen and oxygen which may serve as the basis for modeling physical and chemical processes in streamer plasma discharges in air. A multi-term theory for solving the Boltzmann equation and a Monte Carlo simulation technique are used to investigate transport and to obtain exact transport coefficients and spatially resolved transport data. Values and general trends in the profiles of the mean energy, drift velocity, diffusion coefficients and rate coefficients are reported.

1. Introduction

Streamers are growing filaments of weakly-ionized non-stationary plasma produced by an ionization front that moves through non-ionized matter. Streamer plasma discharges have long been of interest, with many scientific and technological applications. They are used in industrial applications such as lighting [1] or gas and water purification [2] and in microelectronics for plasma enhanced vapor deposition [3]. Streamers also occur in natural phenomena. They play a crucial role in creating the paths of sparks and lightning [4]. Sprites, blue jets and other transient luminous events in the upper atmosphere can also be related to streamers. Recent telescopic images of sprites have revealed that they are composed of a multitude of streamers [5]. Therefore accurate modeling and simulation of streamers is of high interest.

The basic microscopic ingredients for a streamer plasma discharge are the following: (1) the generation of electrons and ions in regions of high electric field; (2) drift and diffusion in the local electric field; and (3) the modification of the externally applied field by the generated space charges [4]. A number of methods to treat these problems have been developed and have been applied to a variety of realistic multidimensional configurations, e.g., fluid and hybrid modeling (see for example Ebert *et al.* [4] and references therein), Monte Carlo collision technique and 3D dielectric breakdown models for the branched streamer trees [6]. In particular, fluid models and/or fluid parts of hybrid models of streamers often require swarm transport coefficients as a function of electric field strengths. As an illustrative example, in a recently developed three-dimensional hybrid model of a streamer plasma discharge [7] the low-energy electrons in the collision dominated plasma region are treated using a fluid model while the fast non-equilibrium electrons in the leading part of the ionization front are treated by a Monte Carlo simulation. The fluid part is based on the local field approximation and requires the tabulation of electron transport coefficients as a function of the reduced electric field. The fluid model is coupled with the Monte Carlo model via a model interface. To ensure the stable and correct interaction between these two models, the correct implementation of swarm transport data and the accuracy of their calculations are critical steps in modeling. In this context, care must be taken when ionization and attachment are operative to ensure that calculated data are an appropriate input in fluid models of streamer plasma discharges. In this work, electron transport coefficients and spatially resolved transport data required for modeling streamers are calculated from solutions of the non-conservative Boltzmann equation and from Monte Carlo simulations.

2. Theory

The governing equation describing a swarm of charged particles moving through a background of neutral molecules in electric and magnetic fields is given by Boltzmann's equation for the phase space distribution function $f(\mathbf{r},\mathbf{c},t)$:

$$\frac{\partial f}{\partial t}+\mathbf{c}\cdot\frac{\partial f}{\partial \mathbf{r}}+\frac{e}{m}\mathbf{E}\cdot\frac{\partial f}{\partial \mathbf{c}}=-J(f). \qquad (1)$$

Here **r** and **c** denote, respectively, the position and velocity of the swarm particle at time *t*, *e* and *m* are the charge and mass of the swarm particle, respectively, while **E** is the electric field. The right hand side of (1) denotes the linear charged-particle-neutral molecule collision operator, accounting for elastic, inelastic, and non-conservative collisions.

The directional dependence of $f(\mathbf{r},\mathbf{c},t)$ in velocity space is represented by an expansion in terms of spherical harmonics:

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

where $Y_m^{[l]}(\hat{c})$ are spherical harmonics and $\hat{c}$ denotes the angles of **c**. No restrictions are placed on the number of spherical harmonics nor is any particular form of the time-dependence of the expansion coefficients assumed. The speed dependence of the coefficients $f(\mathbf{r},c,t)$ is treated by

an expansion about a Maxwellian at an arbitrary time-dependent basis temperature in terms of Sonine polynomials. It is assumed that the hydrodynamic stage has been reached and that spatial dependence is treated by the density gradient expansion:

$$f(\mathbf{r},\mathbf{c},t)=\sum_{s=0}^{\infty} f^{(s)}(\mathbf{c},t)\otimes(-\nabla)^s\, n(\mathbf{r},t). \qquad (3)$$

Using the above decompositions of f and an implicit finite difference evaluation of time derivatives, the Boltzmann equation is transformed into a hierarchy of doubly infinite coupled inhomogeneous matrix equations for the time-dependent moments. Finite truncation of both the Sonine polynomial and spherical harmonic expansions permit solution of this hierarchy by direct numerical inversion. Having obtained the moments, the transport coefficients and other transport properties can be calculated and their explicit expressions are given by Dujko *et al.* [8].

3. Results and discussion

We consider the reduced electric field range: 1-1000 Td (1 Td = 10^{-21} Vm^2). The abundance of O_2 in the mixture is varied systematically. The cross sections for the electron scattering in N_2 detailed by Stojanović and Petrović [9] and cross sections for electron scattering in O_2 developed by Itikawa *et al.* [10] are implemented in this work.

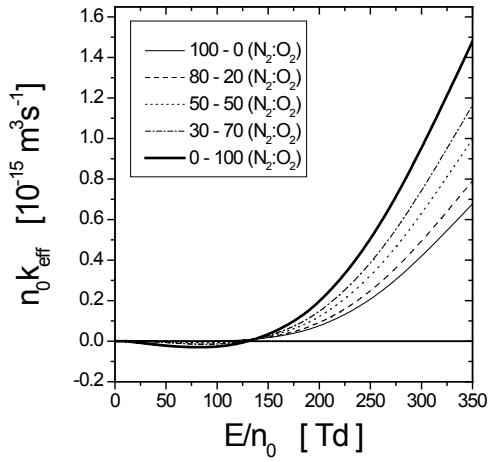

Fig.1. Variation of the effective ionization coefficient with E/n_0 for various N_2-O_2 mixtures.

Fig. 1 displays the variation of the effective ionization coefficient with E/n_0 for various N_2-O_2 mixtures. For clarity, we show the variation of n_0k_{eff} with E/n_0 up to 350 Td. For E/n_0 less than ~135 Td and when O_2 is present, n_0k_{eff} is negative, although its value is relatively small. This is a clear sign that the attachment dominates the ionization in this energy region. However, due to the increasing cross section for ionization and the fact that the cross section for electron attachment becomes negligible at higher energies, the effective ionization coefficient becomes positive. A very narrow range of E/n_0 where the effective ionization coefficient passes through zero is of special interest for modeling of streamers, since it corresponds to the minimal value for the development of an electron avalanche and its transition into a streamer.

As an illustrative example how to model spatiotemporal development of the swarm and the growth of the total electron avalanche, in Fig. 2 we show the spatial distribution of an electron swarm for various N_2-O_2 mixtures obtained by Monte Carlo simulations. The applied electric field is set to 590 Td. The electron swarm is released at time $t = 0$, from a single point with a Maxwellian distribution of velocities and with a mean starting energy of 25 eV. As can be observed, the spatial density profiles of the swarm relax to a typical Gaussian profile after a sufficient spatial segregation. We observe that the spatial development of the swarm is significantly affected by the amount of O_2 in the mixture.

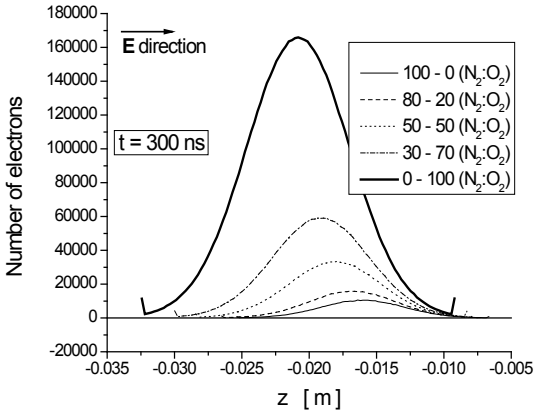

Fig. 2. The spatial distribution of the electron swarm for various N_2-O_2 mixtures.

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