Modelling of an atmospheric pressure dc glow discharge

P. Simon(*)[1], A. Bogaerts[1]

[1] *Research Group PLASMANT, Department of Chemistry, University of Antwerp, Universiteitsplein 1, 2610 Wilrijk-Antwerp, Belgium*

(*) peter.simon@ua.ac.be

A two-dimensional hydrodynamic model is used to simulate an atmospheric pressure helium glow discharge in a pin to plate type geometry. A self-consistent description is used including the effect of space charges, heating and gas flow. The results include two-dimensional profiles of electric potential, temperature and densities of several plasma species as well as the velocity field of the gas flow. The results of the simulations are compared with experimental data. The effect of nitrogen impurities is also investigated.

Introduction

Atmospheric pressure glow discharges (APGDs) are gaining increasing interest in recent years. The elevated pressure applied in these discharges liberates from the need of expensive vacuum systems and extends the potential application area of glow discharges (GDs) to non-vacuum compatible materials and processes. To optimize the applications of APGDs, a thorough characterization of the high pressure GD plasma is desirable. In spite of the great interest, the fundamental mechanisms of many APGDs have not been fully understood yet, which is mainly due to the complexity of physical-chemical processes.

We have started the systematic study of a direct current glow discharge established between a pin and a plate electrode in an atmospheric pressure helium gas. This discharge is used in the flowing afterglow mode as an ambient chemical ionization source for organic mass spectrometry [1]. The characterization of the discharge by means of computer modelling requires a self-consistent description including the effect of space charges as well as the heating and the gas flow. In the present study we also investigate the effect of nitrogen impurities and the simulation results are compared with experimental data.

Description of the model

We used the two-dimensional model, called *nonPDPSIM*, which was developed in the research group of Mark J. Kushner [2].

A continuity equation is solved for each plasma species:

$$\frac{\partial n_j}{\partial t} = -\vec{\nabla}\cdot\vec{\Gamma}_j + S_j, \tag{1}$$

where n_j is the density, $\vec{\Gamma}_j$ is the flux and S_j is the source function of species j. The flux can be written as

$$\vec{\Gamma}_j = n_j\vec{v} + n_j\mu_j\vec{E} - D_j\vec{\nabla}n_j, \tag{2}$$

where $\vec{E}$ is the electric field, μ_j is the mobility (it is zero for neutrals and negative for negatively charged species) and D_j is the diffusion coefficient of species j. The advective velocity $\vec{v}$ describes the bulk motion of the gas and is obtained from the solution of the system of Navier-Stokes equations.

The electrical potential is calculated by solving Poisson's equation:

$$-\vec{\nabla}\cdot(\varepsilon\vec{\nabla}\phi) = \sum_j n_j q_j + \rho_m, \tag{3}$$

where ε is the permittivity, ϕ is the electric potential, q_j is the charge of species j and ρ_m is the charge density originating from charge accumulation on the boundary of the plasma and a dielectric material.

The electron temperature (T_e) is obtained by solving an energy balance equation for the bulk electrons:

$$\frac{\partial(n_e \varepsilon_e)}{\partial t} = q_e \vec{\Gamma}_e \cdot \vec{E} - n_e \sum_j n_j k_j \Delta\varepsilon_j - \vec{\nabla} \cdot \left(\frac{5}{3} \varepsilon_e \vec{\Gamma}_e - \lambda_e \vec{\nabla} T_e \right), \tag{4}$$

where ε_e is the average electron energy ($\varepsilon_e = \frac{3}{2} k_B T_e$) and λ_e is the electron thermal conductivity. The sum on the right side of the equation accounts for the energy change ($\Delta\varepsilon_j$) of the electrons in collisions with species j with a rate coefficient k_j. The secondary electrons emitted from the cathode (and their progeny) are followed by a Monte Carlo (MC) model until they slow down sufficiently to be treated by the continuum model.

The above equations are solved on an unstructured mesh. In order to reach a steady state solution, processes having vastly disparate timescales have to be coupled to each other, which is achieved by using time-slicing techniques [3].

Results

The species included in the model are He, He^*, He_2^*, He^+, He_2^+, N_2, N, N_2^+, N^+, e^-. The discharge current and the gas flow rate are set to 25 mA and 1500 sccm, respectively. Note that only preliminary results are shown in Fig. 1, because the steady state solution has not been reached yet.

Fig. 1(a) shows the streamlines of the gas flow and the contour lines of the temperature. The gas enters parallel to the pin cathode from the bottom and flows out through an orifice located in the centre of the disk anode. The experimental value of the temperature is 1170 K at the tip of the pin cathode and roughly constant at around 770 K in the positive column [4].

Fig. 1(b) shows the relative contribution of nitrogen ions (N^+ and N_2^+) to the total ion density. It is clear that although only 10 ppm N_2 enters into the discharge with the gas flow, the positive column is dominated by nitrogen ions (>80%), which are generated effectively via charge transfer and Penning ionization.

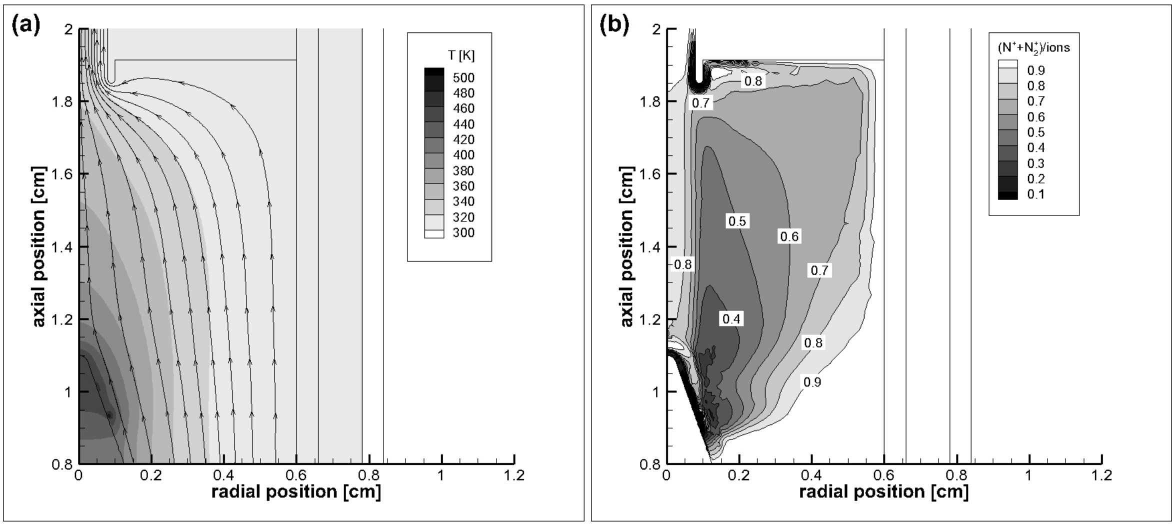

Fig. 1: (a) Streamlines of the gas flow and contour lines of temperature. (b) Relative contributions of nitrogen ions (N^+ and N_2^+) to the total ion density.

References

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