Mohammed BOUKABBOUT, Ben-Yssaad KRALOUA, Ali HENNAD
Université des Sciences et de la Technologie d'Oran Mohamed BOUDIAF USTO-MB, FGE, BP 1505 El M'Naouer, 31000 Oran, Algerie

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DC glow discharge modelling by using electrons transport parameters from the BOLSIG+ code

***Abstract**. The fluid model used for the discharge simulation in argon gas require the electron and ionic transport parameters. These parameters transport for electrons are calculated from collisions cross sections data by solving the Boltzmann equation in the Bolsig+ code. For ionic transport parameters are from Ellis et al. compilation. In this work, we present the one dimensional modeling of the DC glow discharge at low pressure and maintained by secondary emission at cathode. The aim this article is to compare our calculations with the research work of Lin and Adomaitis. This two authors have used the constant transport parameters for electrons and ions (independent of electric field and electron energy).*

Streszczenie**. W modelu cieczowym do symulacji wyładowania w argonie wymagana jest znajomość parametrów transportu jonowego. Parametry transportu elektronowego określane są na podstawie równania Bolsiga. Transport jonowy obliczany jest na podstawie modelu EWllisa. W artykule opisano modelowanie wyładowania DSC w gazie o niskim ciśnieniu. Wyniki porównano z rezultatami prezentopwanymi przez innych autorów. **Modelowanie wyładowania DC na podstawie parametrów transportu z równania BOLSIG+.

Keywords: Fluid model, DC glow Discharge, Bolsig+ code.
Słowa kluczowe: wyładowanie DC, kod BOLSIG

Introduction

In a DC glow discharge, the electric field is homogeneous in the inter-electrode space. The ions striking the cathode create secondary electrons. The electron avalanche creates much electron that ions but electrons being 100 times faster than ions, they drift quickly to the anode where they are absorbed. The ions having a lot of inertia accumulate in the inter-electrodes space, then the number of ions accumulates increases and from an accumulation threshold, the electric field is no longer homogeneous while it decreases on the side anode, which has the effect of slowing the electrons that drift towards the anode. The process continues until the electric field at the anode vanishes. The electrons can no longer pass freely to the anode and are considerably slowed down. The electron number density increases until to equal of the density of ions. A plasma is formed near the anode. The number of charged particles increases and the plasma extends from the anode to the cathode. The extension of the plasma compresses the region of strong field towards the cathode. These phenomena continue until the creation of charged particles is equilibrate (creation=losses). Two regions appear, the sheath and the plasma.

The majority of electric discharge in gases (plasma) are built upon the Boltzmann equation. In principle, the combination of the Boltzmann equation, together with the Maxwell equations, needed for computation of the electromagnetic field, describes the physics of many discharges completely provided that this set of equations is equipped with suitable boundary conditions. In practice, however, the Boltzmann equation is unwieldy and cannot easily be solved without making significant simplifications.

Fluid models describe the various plasma species in terms of average hydrodynamic quantities such as density, momentum and energy density. These quantities are governed by the first three moments of the Boltzmann equation: continuity, momentum and energy balance equation. A more general fluid approach is the multifluid approach, based on the fact that the electrons behave differently from the atoms, molecules or ions and the species are treated separately. In general, the self-consistent system is closed by Poisson's equation describing the electrostatic field and by Maxwell's equations describing the electromagnetic field.

In order to determine the glow discharge characteristics, we need the transports parameters.

The main utility of BOLSIG+ code is to obtain electron transport coefficients and collision rate coefficients from more fundamental cross section data.

DC glow discharge model equations

The continuity equation for species p has the expression [2]:

$$\frac{\partial n_p}{\partial t}+\frac{\partial \Gamma_p}{\partial x}=S_p \tag{1}$$

where $p=i$ or e are index respectively for ions and electrons. In this model, the discharge is sustained by electron impact ionization and electron secondary emission. The former is integrated in the source term S_p, which is given by:

$$S_p=k_{ion}n_g n_e \tag{2}$$

where k_{ion} is the ionization rate coefficient; and the latter is reflected in boundary conditions, n_g is the neutral species density and n_e is the electron density and.

The flux Γ_p is given by the momentum balance equation, which is usually approximated by the drift–diffusion equation

$$\Gamma_p=\pm\mu_p n_p E-D_p\nabla n_p \tag{3}$$

where n_p, μ_p, E, D_p and ∇n_p are respectively the density, mobility, electric field, diffusion and the density gradients of the species p.

The first term represents the flux due to the electric field (drift) and the second is the flux due to density gradients (diffusion). In this paper, the sign of the electron mobility is negative (-) and positive (+) for reduced mobility.

The electron diffusion temperature dependent is given by the following expression:

$$D_e=\mu_e k_B T_e / q \tag{4}$$

where q is the charge of species ($q=1.6022\ 10^{-19}$ (Cb)), T_e is the electron temperature, μ_e is the electron mobility and k_B is the Boltzmann constant ($k_B=1.38062\ 10^{-23}$ (J/°K)).

The electron energy is determined by solving the electron energy balance equation

$$\frac{\partial n_\varepsilon}{\partial t}+\frac{5}{3}\frac{\partial \Gamma_\varepsilon}{\partial x}=S_\varepsilon \tag{5}$$

where $n_\varepsilon = n_e \varepsilon_e$ is the electron energy density. The energy source term S_ε is given by

$$S_\varepsilon = -q\ \Gamma_e E - k_{ion} H_{ion} n_g n_e - K_{loss} n_g n_e \tag{6}$$

where H_{ion} is the ionization enthalpy loss and K_{loss} is the energy loss coefficient.

The flux of electron energy density can be written as:

$$\Gamma_\varepsilon = -\mu_e n_\varepsilon E - D_e \frac{\partial n_\varepsilon}{\partial x} \tag{7}$$

The electric field can be denoted as the negative gradient of the potential:

$$E = -\frac{\partial V}{\partial x} \tag{8}$$

Boundary conditions

The transport equations as well Poisson's equation can be solved only if boundary conditions are specified. For Poisson's equation, the boundary conditions include the fact that the anode is grounded (*V_{anode} = 0*) and that a negative voltage *$V_{cathode}$* =-*V_{DC}* is applied to the cathode (see figure 1).

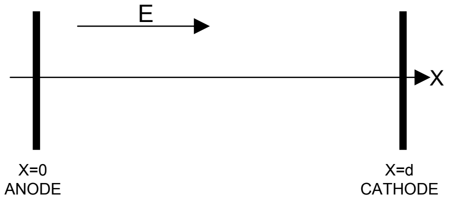

Fig. 1: The 1D geometry of DC glow discharge used for the simulation.

For our fluid model, the boundary conditions at the grounded electrode (x = 0) are given as follow:

$$V=0\,; \qquad n_e=0\,; \qquad \nabla n_i = 0$$

$$\frac{5}{2}\nabla T_e - \frac{q}{k_b}\nabla V = 0$$

And at the powered electrode (*x* = *d*):

$$V=-\,V_{DC}\,; \qquad \nabla n_i = 0\,; \qquad T_e = T_{ec}$$

The secondary electron emission by ion bombardment at the cathode constitutes the most important process. It is described by the relation of the electron and ion flux.

$$\Gamma_e = -\gamma\,\Gamma_i \tag{9}$$

where γ is the secondary electron coefficient.

Numerical methods

In this section, for calculation the densities charged particles, the continuity equation (1) must be solved.

The transport equation for electronic energy (5) has the same form as equation (1), by changing the particles density n_e with the average electrons energy density n_ε and by correctly expressing the source term S_ε.

So the form of the transport equation to be solved is expressed as follows:

$$\frac{n_{pk}^{m+1}-n_{pk}^{m}}{\Delta t}+\frac{\Gamma_{pk+1/2}^{m}-\Gamma_{pk-1/2}^{m}}{\Delta x}=S_{pk}^{m} \tag{10}$$

The drift-diffusion fluxes are discretized using the Scharfetter-Gummel exponential scheme [3].

$$\Gamma_{pk+1/2}^{m}=\frac{D_{pk+1/2}}{\Delta x^{+}}\frac{R_1}{1-e^{R_1}}n_{pk+1}^{m}-\frac{R_1\ e^{R_1}}{1-e^{R_1}}n_{pk}^{m} \tag{11}$$

$$\Gamma_{pk-1/2}^{m}=\frac{D_{pk-1/2}}{\Delta x^{-}}\frac{R_2}{1-e^{R_2}}n_{pk}^{m}-\frac{R_2\ e^{R_2}}{1-e^{R_2}}n_{pk-1}^{m} \tag{12}$$

with

$$R_1=\mu_{pk+1/2}\ E_{k+1/2}^{m}\ \Delta x^{+}\ /\ D_{pk+1/2}$$

$$R_2=\mu_{pk-1/2}\ E_{k-1/2}^{m}\ \Delta x^{-}\ /\ D_{pk-1/2}$$

$$\Delta x^{-}=x_i-x_{i-1}$$

$$\Delta x^{+}=x_{i+1}-x_i$$

For the calculation of the field and potential electric, we are used discretization of Poisson's equation as follows:

$$\frac{\partial^2 V}{\partial x^2}=\frac{q}{\varepsilon_0}(n_e-n_i)\ =\ \frac{V_{k+1}-2V_k+V_{k-1}}{\Delta x^2} \tag{13}$$

where $\varepsilon_0 = 8.85\ 10^{-12}$ (F/m) is the permittivity of free space.

The resulting linear system is then solved using the tri-diagonal method.

Results and discussions

the discharge simulation is carried in argon gas for a temperature 300 (° K). A parallel plate configuration is used for the glow discharge; the inter-electrodes distance is 3.525 cm as shown in figure (1). The transport parameters have been taken from [4], [5] and [7].

The electron mobility, ionization rate coefficient and the energy loss coefficient are functions electron mean energy and they are obtained from the solver BOLSIG+ [5] (see figure (2)) using cross-section data for argon [6]. For ions, the mobility and the diffusivity are a function reduced electric field, we have used the data compilation given by Ellis et *al.* [7] (see figure (3)). The electron diffusion coefficient is calculated from the Einstein relation (4). The following table (1) contains all the data and transport parameters used in our one-dimensional modeling.

Table 1: Gas physical properties and glow discharge system dimensions [4] [5] [7] [8].

Symbol	***Description***	***Value***
d	*Inter-electrodes spacing*	*3.52 5 cm* [4]
n_g	*Neutral species density*	*2.83 10^{16}cm^{-3}* [4]
D_e	*Electron diffusion*	*Einstein relation* [4]
D_i	*Ion diffusion*	*Data Ellis* [7]
μ_e	*Electron mobility*	*Bolsig+* [5]
μ_i	*Ion mobility*	*Data Ellis* [7]
H_{ion}	*Ionization enthalpy loss*	*15.578 eV* [4]
γ	*Secondary electron coefficient*	*0.046* [4]
V_{DC}	*Direct current voltage*	*77.4 v* [4]
K_{ion}	*Ionization rate prefactor*	*Bolsig+* [5]
K_{loss}	*Energy loss coefficient*	*Bolsig+* [5]
T_{ec}	*Electron temperature at cathode*	*0.5 eV* [4]

The results obtained from our 1D code of glow discharge characteristics in stationary state such as densities electron and ion, electric potential, electric field and electron temperature as a function inter-electrodes distance are represented in the figures 4 to 7.

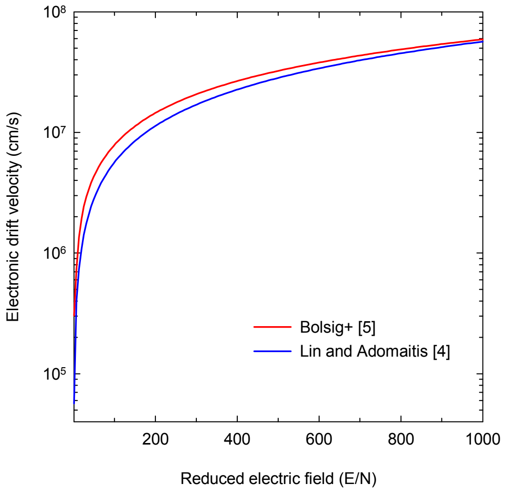

Fig. 2: Electron drift velocity as a function the reduced electric field.

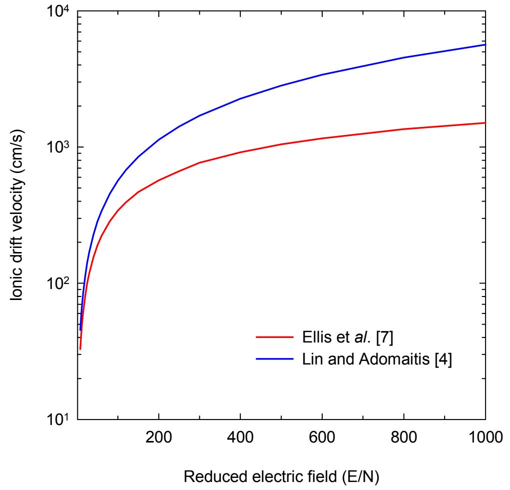

Fig. 3: Ion drift velocity as a function the reduced electric field.

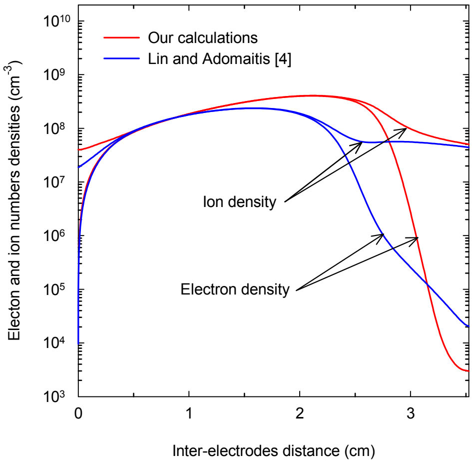

Fig. 4: Electron and ion number densities distributions.

In the cathodic region, we notice that there are differences between our calculations and those obtained by Lin and Adomaitis [4]. In this region of the glow discharge, the electric field and electron temperature are relatively intense. In our calculations, the transport parameters are given according to the values of the electron temperature and the electric field. In the calculations of these two authors, the transport parameters are independent of the electron energy value, although indeed a numerical code based on the second order fluid model. In the figure (2), the electron drift velocity from the Bolsig+ code is relatively high compared to that used by Lin and Adomaitis [4]. This is the reason why the electrons gain more energy to make ionization collisions in the cathodic region. This production process of charged species will influence the density values and the other glow discharge characteristics.

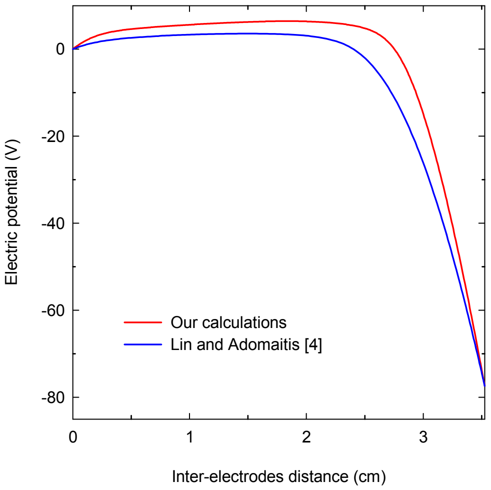

Fig. 5: Electric potential distributions.

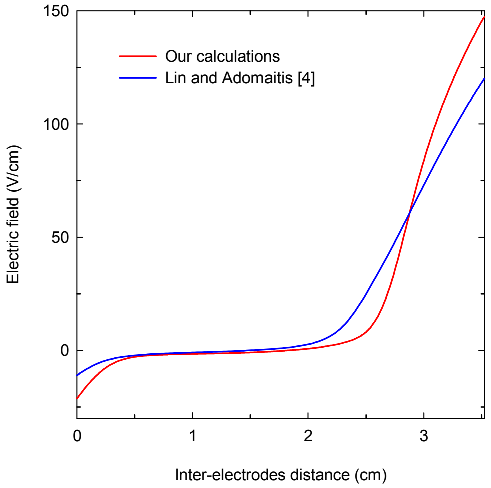

Fig. 6: Electric field distributions.

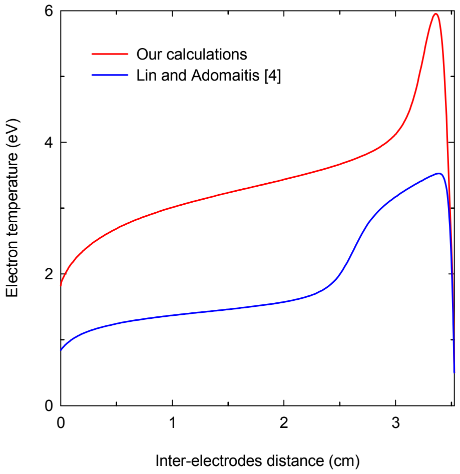

Fig. 7: Electron temperature distributions.

Conclusion

In this paper, we have presented the one-dimensional model of glow discharge at low pressure and comparing our calculations derived from the transport parameters used by

Lin and Adomatis [4] and that obtained by solver Bolsig+ [5]. Our results are relatively in good agreement with those of Lin and Adomatis [4], except in the cathodic region of the electric discharge. The aim of this work was to determine the characteristics of glow discharge using the variable transport parameters (as a function of the reduced field E/N and the electronic temperature).

Authors: *Mohammed Boukabbout was born in Mostaganem, Algeria, on December, 13, 1988. His scientific interests include the plasma engineering and the theoretical study and modeling of the DC glow discharge,* E-mail: m.boukabbout@yahoo.fr
Ali Hennad was born in Oran, Algeria, on January, 27, 1964. He received the PH.D degree with a thesis on the kinetics of ions in molecular gases to determine ion basic data in air form Monte Carlo simulation, University Paul Sabatier of Toulouse, France in 1996. He is currently a Professor at University of Sciences and Technology of Oran, Algeria. His field of expertise is more particularly the modeling of the electric and hydrodynamic behaviors of the plasmas generated in low and high pressure. He has also a good expertise on the numerical analysis of the nonlinear and strongly coupled elliptic transport equations, and the swarm parameters determination of the charged particles in no equilibrium reactive plasma. He is the author of various international publications, a lot of them in collaboration with the LAPLACE Laboratory, Toulouse, France, E-mails: ali_hennad@yahoo.fr

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