Two-dimensional hybrid model for a glow discharge: comparison with fluid and kinetic (particle) models, reliability and accuracy

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Abstract. We developed and tested a two-dimensional Monte Carlo – fluid hybrid numerical code for the DC glow discharge simulations. The model is based on the separation of electrons into two parts, namely, the low energetic (slow) and high energetic (fast) groups. Ions and slow electrons are described within the fluid model using the drift-diffusion approximation for particle fluxes. Electrostatic field is obtained from the solution of Poisson equation. Fast electrons, represented by the appropriate number of super particles emitted from the cathode, are responsible for ionization processes in the discharge volume. Test calculations were carried out for the argon plasma. The vortex current formation in a DC discharge is observed in the case of rectangular geometry.

1. Introduction
The physics of gas discharge phenomena, natural or man-made, is based on the dynamics of electrons and ions, created by the ionization of neutral gas particles. Gas discharges demonstrate certain nonlinear properties, among which the formation of sheath layers near the electrodes, existence of specific regions inside the discharge volume glowing with different intensities, secondary electron emission from electrodes by the impact of energetic charged particles. Furthermore, nonlocal transport characteristics of electrons in high electric field regions make this phenomena complicated to investigate. Numerical modeling techniques used to study the gas discharges include fluid, hybrid, and kinetic (particle) methods [1, 2]. Within the fluid method, the particle species (electrons, ions, and neutrals) are considered as fluids described by the continuity equations with drift-diffusion approximation for particle fluxes. Fluid models usually employ a local field approximation (LFA), according to which transport coefficients as well as the ionization rate are determined as functions of the reduced electric field [3, 4, 5]. Fluid methods in general are capable to describe basic qualitative properties of plasma. Within the kinetic (particle) methods, which provide quantitatively accurate results, particle species are simulated by the suitable number of super particles [6, 7, 2]. Hybrid methods are partially fluid and partially kinetic [8, 9, 10, 11].

In this work we present a two-dimensional Monte Carlo – fluid hybrid model for a rectangular discharge geometry filled with argon gas. The details of the model are described in section 2. Numerical results and discussion are presented in section 3. Finally, in section 4, a brief summary of the study is given.
2. Model

The model is based on separation of the electrons into two groups, namely, the low energetic (slow) and high energetic (fast) electrons [12]. Ions and slow electrons are described within the fluid model using drift-diffusion approximations for particle fluxes [4]. Electric field is obtained from solution of the Poisson equation. Dynamics of fast electrons and the effect of collisions are simulated by the Monte Carlo Collision (MCC) method that allows to take the nonlocal transport of electrons in the cathode region properly into account [12, 9]. Fast electrons are responsible for ionization processes in the discharge volume. These are simulated by a suitable number of super particles (e.g. 500) emitted from cathode into the discharge volume. Electron elastic, excitation and ionization collisions with the background neutral gas particles are included in the model, while the electron–electron and electron–ion collisions are ignored. The occurrence, type and scattering angles of the collisions are determined by random numbers uniformly distributed between 0 and 1.

2.1. Fluid model

Fluid model includes continuity equations for electrons and ions [13],

\[
\frac{\partial n_e}{\partial t} + \nabla \cdot \mathbf{\Gamma}_e = S_e, \tag{1}
\]

\[
\frac{\partial n_i}{\partial t} + \nabla \cdot \mathbf{\Gamma}_i = S_i, \tag{2}
\]

coupled with the Poisson equation for the electric field,

\[
\nabla^2 V = -\frac{e}{\varepsilon_0} (n_i - n_e). \tag{3}
\]

Here \( n \) denotes the particle density, \( \mathbf{\Gamma} \) the flux density, \( V \) the electric potential. Subscripts \( e \) and \( i \) refer to electrons and ions. \( S \) the ionisation source term obtained from the MCC simulation of fast electrons. Flux densities are expressed in the drift-diffusion form [4],

\[
\mathbf{\Gamma}_{i,e} = -D_{i,e} \nabla n_{i,e} \pm \mu_{i,e} \mathbf{E} n_{i,e}, \tag{4}
\]

where \( D \) is the diffusion coefficient, \( \mu \) the mobility coefficients, and \( \mathbf{E} \) the electric field vector.

2.2. MCC Simulation of Fast Electrons

The fast electrons are traced in the discharge volume as they move in the electric field and make random collisions (elastic or inelastic) with the background neutral gas atoms. The velocities \( \mathbf{v} \) and positions \( \mathbf{r} \) of these particles between collisions are obtained by using dynamical equations,

\[
\mathbf{v}^{k+1}_i = \mathbf{v}^k_i + \mathbf{a}^k_{eff,i} \Delta t, \tag{5}
\]

\[
\mathbf{r}^{k+1}_i = \mathbf{r}^k_i + \mathbf{v}^k_i \Delta t + \frac{1}{2} \mathbf{a}^k_{eff,i} \Delta t^2. \tag{6}
\]

Here indices \( i \) and \( k \) refer to the \( i \)'th electron and the time level. \( \Delta t \) is the time step size. In the case of one-dimensional motion effective acceleration \( \mathbf{a}_{eff} \) is determined from

\[
\mathbf{a}_{eff} = -\frac{e}{m_e} (\mathbf{E} + \frac{1}{2} v_x \Delta t \frac{d \mathbf{E}}{dx}). \tag{7}
\]

Here \( e \) is the electron charge, \( m_e \) the electron mass, \( E \) the electric field magnitude, and \( v_x \) the \( x \) component of the velocity.
Figure 1. Elastic, excitation, ionization and total cross-sections for electrons in argon gas [14].

For a small time step $\Delta t$ the collision probability of electrons is expressed in the form

$$P_c = 1 - e^{-N_g \sigma_{tot}(v_r) v_r \Delta t},$$

(8)

$$\sigma_{tot} = \sigma_{el} + \sigma_{ex} + \sigma_{iz},$$

(9)

where $N_g$ is background neutral gas density, $\sigma_{tot}$ is velocity (or energy) dependent total collision cross section, $v_r$ is a relative velocity. The cross-section set is presented in figure 1. For the collisions between fast electrons and neutral gas particles, these velocities coincide with the electron velocities. For a group of electrons, the probability of collisions can be obtained by averaging over distribution and expressed in the form

$$P_c = 1 - e^{-N_g \langle \sigma_{tot}(v) v \rangle dt}.$$  

(10)

When multiplied with the total number of electrons in the simulation, this probability gives the total number of electrons that collide with the background gas atoms. The criterions of making a collision and a specific type of collision (elastic, ionization or excitation) are determined by the random numbers uniformly distributed between 0 and 1 [10, 2]. After all fast electrons within MCC cycle have escaped from the volume or converted to the slow electrons, the ionization events data is interpolated into the grid points in order to determine the ionization rate profile. The ionization source profile is weighted to the actual value using the equation [11, 17]

$$S_{i,e} = \frac{j}{(1 + 1/\gamma) \Delta x} \frac{N_{i,e}}{N_0},$$

(11)

where $j$ is the electric current density at the cathode, $\gamma$ the secondary electron emission coefficient, and $\Delta x$ the grid cell size. $N_{i,e}$ are the ionization profiles obtained from MCC cycle. $N_0$ is the initial number of super electrons emitted from cathode in the MCC cycle.

2.3. Geometry and Boundary Conditions
The calculations are carried out in the a rectangular region with a uniform grid in each direction. Cathode and anode locate at the left and right border respectively.

Boundary condition for the electric potential are the grounded potential on the cathode and applied voltage $V_a$ on the anode. On the dielectric side walls, which are perfect absorbers, electric field is determined by the Gauss law, $\mathbf{n} \cdot \mathbf{E} = -\sigma/\varepsilon_0$. The charge accumulation process is expressed by the equation

$$\frac{d\sigma}{dt} = e(\Gamma_i - \Gamma_e) \cdot \mathbf{n},$$

(12)
where \( \sigma \) is the surface charge density, \( \hat{n} \) is outward normal to the wall surface.

Boundary conditions for particle species on the electrodes and side walls are given by the directed fluxes. For electrons \([15]\),

\[
\hat{n} \cdot \Gamma_e = \frac{1}{4} n_e v_e - \alpha_e \mu_e n_e (\hat{n} \cdot E) - \beta_e \gamma |\hat{n} \cdot \Gamma_e|,
\]

and for ions,

\[
\hat{n} \cdot \Gamma_i = \frac{1}{4} n_i v_i + \alpha_i \mu_i n_i (\hat{n} \cdot E).
\]

Here, \( v_{i,e} = \sqrt{8\pi T_{i,e}/m_{i,e}} \) are the electron and ion thermal speeds. The last term in equation (13) describes the secondary electron emission from the walls bombarded by energetic ions, \( \beta_e = 1 \) on cathode and 0 otherwise. \( \alpha_{i,e} \) controls the directed convective fluxes to the walls: it equals 1 if the flux is directed into the wall and 0 otherwise.

2.4. Plasma Parameters

Model is simulated in argon gas at pressure \( p = 1 \) Torr with a constant temperature \( T_g = 0.025 \) eV. \( L_x = 1 \) cm and \( L_y = 1 \) cm. We used constant transport coefficient for slow electrons, \( \mu_e = 3 \times 10^5 \text{ cm}^2\text{s}^{-1}\text{V} \) and \( D_e = \mu_e T_e \), where \( T_e = 1 \) eV \([17]\). Ions are assumed to be in thermal equilibrium with background gas, \( T_i = T_g = 0.025 \) eV. Mobility and diffusion coefficients of ions are determined as functions of reduced electric field as in Ref. \([16]\) and \([18]\).

3. Numerical Results and Discussion

3.1. 1D Results: Comparison and Validation

We compared our 1D simulation results (electron density, electric field and ionization source profile) in figure 2 with results of Ref. \([17]\). For electrons and ions zero density boundary conditions are used on the anode, zero gradient for ions and secondary electron emission condition for electrons on the cathode. Results are in good agreement. Figure 2 contains also fluid model results obtained under the same parameter regime. Results show that fluid method cannot predict correctly the charged particle densities, electric field, and ionization source profile. Moreover, the field reversal, which occurs at \( x = 0.36 \) cm within the hybrid model, is not obtained by the fluid model.
3.2. 2D Results

**Figure 3.** 2D hybrid model. (a) electron density (colored) and current flow (white streamlines), (b) ion density (logarithmic scale) and current flow, (c) fast electron density and current flow. $p = 1$ Torr, $T_e = 1$ eV, $\gamma = 0.06$, $L_x = 1$ cm, $L_y = 1$ cm, $V_a = 250$ V.

2D hybrid model results are presented in the figure 3. As can be seen from the electron and ion density profiles in panels 3a and 3b, strong domination of electron flux directed to the walls over the ions flux leads to formation of sheath reagins near the walls. Maximum density values locate on the symmetry axis as expected. The potential and electric field profiles represent a usual pattern on the cathode region with a high voltage drop and electric field in this region.

3.3. Electric Current Flows

**Figure 4.** Electric current densities of electron and ions. (a) 1D, (b) axial profiles in 2D, (c) transversal profile through point $x = 0.5$ cm in 2D.

An interesting result is presented in figure 3: vortex current formations in the DC discharge. Figure 3a illustrates the total electron current flow, 3b the ion current flow, and 3c the fast electron current flow. The vortex current phenomena was predicted theoretically and identified by using numerical calculations in [19] in the case of an ICP (Inductively Coupled Plasma) discharge. As it follows from figure 3a and 3c, these formations is mostly due to the electron current flow.
Figure 4 represents the electron, ion, and total electric current profiles. Flat line for the total current density in figure 4a supports the correctness of the simulations. The same behaviour occurs in 2D case (figure 4b), disturbed by the fast electron flux in the cathode sheath. Figure 4c demonstrates the nonambipolar behavior of electron and ions currents in the transversal direction.

4. Conclusion
We developed and tested 2D Monte Carlo – fluid hybrid numerical model for a DC glow discharge. 1D calculations were also implemented in order to carry out the validation of the numerical code. Basic properties of glow discharge plasma sustained in argon gas (such as spatial profiles of charged particle densities, electric field, and ionization source) were studied. Simulations showed that the hybrid numerical model with fast electron group responsible for the ionization processes in the volume can be used to describe the nonlocal characteristics of plasmas of DC discharge. Vortex current formations in the total electric current flow were observed.

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