Fluid model of dc glow discharge with nonlocal ionization source term

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Abstract. We developed and tested a simple hybrid model for a glow discharge, which incorporates nonlocal ionization by fast electrons into the fluid framework. Calculations have been performed for an argon gas. Comparison with the experimental data as well as with the hybrid (particle) and fluid modelling results demonstrated good applicability of the proposed model.

1. Introduction

Different approaches that are used for the glow discharge modelling can be classified as fluid models, kinetic (particle) models, and their combinations known as hybrid models (see, e.g., [1]). All the discharge models have their advantages and disadvantages. Advantages of the fluid models are their relative simplicity and computational efficiency. However, these models are very approximate, mainly due to the local field approximation (LFA), in which ionization is assumed to be dependent on the local value of the electric field [2]. Nonlocal ionization is approximately taken into account in the "extended fluid models", in which the electrons are described in terms of the fluid dynamics but their transport and kinetic coefficients are calculated as functions of the electron temperature, through the solution of the local Boltzmann equation (see, e.g., Refs. [3, 4, 5, 6]).

Exact description of the electron behavior can be obtained by solving the kinetic Boltzmann equation [7, 8, 9, 10]. However, this approach is mathematically very complicated, especially if more than one dimension needs to be simulated. Method known as PIC/MCC (Particle in Cell/Monte Carlo Collisions [11, 12]) which couples MC simulations for the behavior of electrons and ions to the Poisson equation for the self-consistent electric field, is also time consuming, and has not come into wide use in the glow discharge plasma modelling.

A compromise between computationally effective but very approximate fluid models and accurate but time consuming particle and kinetic models is represented by hybrid models [5, 11, 13, 14, 15, 16, 17]. These methods are based on separating the electron ensemble into different, independently behaving groups, which cannot be described within the fluid model, which deals with variables averaged over the whole ensemble. Basically, two main groups of electrons are identified. The first group is formed by high energetic (fast) electrons, which emerge as secondary electrons at the cathode surface or are created in the ionization processes in the cathode-fall region. Second group consists of low energetic (slow) bulk electrons, which mainly locate in the quasineutral region of the discharge.
Figure 1. Electron cross sections for (1) elastic, (2) direct ionization, (3) excitation, (4) excitation, and (5) stepwise ionization collisions in argon, used in the model. Curve labels correspond to indices of corresponding processes in Table 1.

Within this approach, slow electrons are responsible mainly for the transport of electron current and provide the balance of plasma density and temperature (mean energy) over the electron ensemble, so they can be described in the framework of the fluid model (simple or extended). Concerning the fast electrons, these are treated as contributing to the ionization processes only and their dynamics are usually described by the Monte Carlo method. This approach is mathematically complicated, and its accuracy is severely limited by poorly known collision cross-sections. At the same time, what is really needed to be known for the discharge description, is such an integral characteristic of the fast electrons as a spatial distribution of the ionization sources, which is then substituted into the balance equations of the ions and plasma electrons. However, in order to find the ionization sources, there is no need to engage in labor-intensive calculations of EDF of fast electrons, accuracy of which is unknown a priori. This characteristic can be approximated analytically and tabulated on the basis of the measured Townsend ionization coefficient or alternatively obtained from the separate MC simulations, and then integrated into the fluid model.

In the context of this approach, in this work, we incorporated effect of fast electrons into the “simple” and “extended” fluid models of glow discharge. Nonlocal ionization source has been formulated in the way first suggested as early as in Ref. [18], and then used in Refs. [2, 19, 20]. We carried out test calculations for the discharge in argon gas, which results were compared with the data obtained from measurements as well as from the “extended fluid” model and hybrid (particle) simulations. Calculations performed showed that the proposed model, which can be called as a simple hybrid model, allows to overcome the shortcomings of the “extended fluid” models, since it takes properly into account the nonlocal ionization in the negative glow. At the same time it is computationally much more efficient compared to the models involving Monte Carlo simulations.

2. Model

2.1. “Simple” fluid model

“Simple” fluid model for the gas-discharge includes continuity equations for the charged and excited particles,

$$\frac{\partial n_k}{\partial t} + \nabla \cdot \Gamma_k = S_k,$$  \hspace{1cm} (1)
which are completed by the Poisson’s equation for the electrostatic field,
\[ \epsilon_0 \nabla \cdot \mathbf{E} = \sum_k q_k n_k, \quad \mathbf{E} = -\nabla \phi. \] (2)

In these equations, subscript \( k \) indicates the \( k \)th species (we will also use subscripts \( i, e, m \) and \( g \) for the ions, electrons, metastable atoms and background gas, respectively), \( n \) stands for the number density, \( S \) denotes the particle creation rate, \( \mathbf{E} \) and \( \phi \) are the electric field and potential, \( q \) is the charge, and \( \epsilon_0 \) is the dielectric constant. \( \Gamma \) denotes the particle flux, which, with parameters \( \mu \) and \( D \) denoting the mobility and diffusion coefficients, is given in the drift-diffusion approximation,
\[ \Gamma_k = sgn(q_k)n_k\mu_k \mathbf{E} - D_k \nabla n_k. \] (3)

Within this model, particle creation rate is determined as function of reduced electric field \( E/p \) ("local field approximation"), which, in general, is an unacceptable approximation (see the discussion in Section 1). In order to remedy the drawbacks associated with the LFA and include, to a certain extent, the nonlocal transport of electrons, "extended" fluid model has been suggested in [3] (which different versions have been applied in Refs. [4, 5, 6]).

2.2. "Extended" fluid model

Within the "extended fluid" model for a glow discharge, the electron transport coefficients (diffusion, \( D_e \), and mobility, \( \mu_e \)) as well as the rates \( S \) of the electron-induced plasma-chemical reactions are calculated as functions of the mean electron energy, \( \bar{\varepsilon} \), rather than the magnitude of the reduced electric field, through the electron energy equation
\[ \frac{\partial n_e}{\partial t} + \nabla \cdot \mathbf{\Gamma}_e = S_e, \]
which is added to the system (1)-(3), and LUT’s ("look-up tables"), obtained from the solution of the local electron Boltzmann equation (see, e.g., Ref. [4]). Here, \( n_e = n_e \bar{\varepsilon} \) denotes the electron energy density, \( \bar{\varepsilon} = 3/2k_B T_e \) is the mean electron energy, and density of the electron energy flux is
\[ \mathbf{\Gamma}_e = -D_e \nabla n_e - \mu_e \mathbf{E} n_e, \] (4)

where energy transport coefficients are related to particle transport coefficients via \( \mu_e = (5/3) \mu_e \) and \( D_e = (5/3) D_e \) [4].

Source function for the electron energy equation has a form \( S_e = P_{heat} + P_{elastic} + P_{inelastic} \), where the first term describes the Joule heating (or cooling) of electrons in the electric field, \( J_{heat} = -e\Gamma_e \cdot \mathbf{E} \), the second term expresses the elastic losses,
\[ P_{elastic} = -\frac{3}{2} \delta \nu_{ea} n_e k_B (T_e - T_g), \]
and the last term is the energy loss in inelastic collisions, \( P_{inelastic} = -\sum_j \Delta E_j R_j \). In these equations, \( \nu_{ea} \) denotes the electron-atomic elastic collision frequency, \( m \) is the particle mass, \( \delta = 2m_e/m_g \), background gas temperature \( T_g = 300 \) K, \( \Delta E_j \) and \( R_j \) are the energy loss (or gain) due to inelastic collision and corresponding reaction rate.

Mobility and diffusion coefficients of heavy particles are approximated by constant parameters, which depends on background gas density, and related by the expression \( D_i/\mu_i = k_BT_i/e \) with \( T_i = T_g \). Electron mobility, \( \mu_e \), and diffusion, \( D_e \), are computed from
\[ \mu_e = -\frac{1}{n_e m_e} \int_0^\infty D_e \sqrt{\varepsilon} \frac{\partial}{\partial \varepsilon} f_0(\varepsilon) \, d\varepsilon, \] (5)
Table 1. Elementary reactions considered in this study. Label Boltz. indicates that constant was calculated from local Boltzmann equation.

| Index | Reaction | Type                  | ΔE (eV) | Constant |
|-------|----------|-----------------------|---------|----------|
| 1     | e + Ar → e + Ar | Elastic collision | 0       | Boltz.   |
| 2     | e + Ar → 2e + Ar⁺ | Direct ionization | 15.8    | Boltz.   |
| 3     | e + Ar ↔ e + Ar⁺ | Excitation | 11.4    | Boltz.   |
| 4     | e + Ar → e + Ar | Excitation | 13.1    | Boltz.   |
| 5     | e + Ar⁺ → 2e + Ar⁺ | Stepwise ionization | 4.4 | Boltz.   |
| 6     | 2Ar⁺ → e + Ar⁺ + Ar | Penning ionization | –       | 6.2 × 10⁻¹⁰ cm³ s⁻¹ |
| 7     | Ar⁺ → hν + Ar | Radiation (including trapping) | –       | 1.0 × 10⁶ s⁻¹ |

\[
D_e = \frac{1}{n_e} \int_0^\infty D_r \sqrt{\varepsilon} f_0(\varepsilon) \, d\varepsilon,
\]

where \( \varepsilon = \frac{mv^2}{2e} \) is the electron kinetic energy (in eV units), \( v \) is the electron velocity, \( D_r = 2\varepsilon/3m_ev_ne \) is the space diffusion coefficient, and \( f_0(\varepsilon) \) is the EEDF obtained from the solution of the local Boltzmann equation.

We used the version of “extended fluid” model applied in [6], where the calculations were performed for an argon gas, and three plasma species, namely, electrons, positive ions, and metastable atoms were taken into account. The set of reactions is given in Table 1, and collision cross-sections are shown in Fig. 1.

Balance of charged particles, in the absence of recombination, is determined by the direct, stepwise, and Penning ionization processes,

\[
S_e = S_i = K_2n_0n_e + K_3n_mn_e + K_6n_m^2.
\]

Here, \( K \) denotes the constant of the corresponding reaction, \( n_0 \) is the concentration of neutral atoms. Reaction constants are numbered according to the list of processes in Table 1. Balance of excited atoms is determined by the reactions of excitation, de-excitation, stepwise ionization, Penning ionization and radiation,

\[
S_m = K_3n_0n_e - K'_3n_mn_e - K_5n_mn_e - 2K_6n_m^2 - K_7n_m,
\]

where \( K'_3 \) is the rate constant of superelastic electron collisions, which correspond to the left-directed arrow for the process 3 in Table 1. Cross-section corresponding to this process is determined by the detailed balance relationship.

For the electron-induced reactions (processes 1–5 in the Table 1), rate constants \( K \) are calculated by convolving the EEDF, obtained from the solution of the local Boltzmann kinetic equation, with the corresponding cross-sections,

\[
K_R = \int_0^\infty \sigma_R(\varepsilon) v(\varepsilon) \sqrt{\varepsilon} f_0(\varepsilon) \, d\varepsilon.
\]

2.3. Models with a nonlocal ionization source.

As we discussed in Section 1, the fast electrons contribution in the hybrid models of glow discharge is limited only to developing the spatial distribution of the ionization (and excitation) rate. Therefore, their effect can be approximated by the analytical formulation of the ionization (and excitation) source function \( S_{\text{fast}} \), and then integrating it into the fluid model.

In the context of this approach, we formulated the nonlocal ionization source in the way suggested in Refs. [2, 19, 20]. The discharge gap is divided into two regions, namely, the
cathode sheath region where the electric field is strong, and the plasma region, where the field is weak. These regions are separated by a point \( x = d \), the sheath boundary, which is determined as a distance \( x \) from the cathode such that the equality \( n_e(x) = 0.5 n_i(x) \) holds. (Due to sharp increase in the electron density in the vicinity of this point and quasineutrality in the plasma, replacing the factor 0.5 in this equation with a number from the range between 0.4 – 0.9 has little effect on the value of \( d \).) Since the ionization source term \( S_{fast}(x) \) decays exponentially with distance from the sheath boundary, it can be approximated as

\[
S_{fast}(x) \propto e^{-(x-d)/\lambda} \quad (x \geq d)
\]

with a decay constant \( \lambda \) [2, 20]. Taking into account that the maximum value of the ionization source is

\[
S_{fast}(d) = \Gamma_e (0) \alpha e^{\alpha d},
\]

where \( \Gamma_e (0) \) is the electron flux density at the cathode and \( \alpha \) is the Townsend ionization coefficient, function \( S \) takes the form

\[
S_{fast}(x) = \begin{cases} 
\Gamma_e (0) \alpha e^{\alpha x} & \text{for } x < d, \\
\Gamma_e (0) \alpha e^{\alpha d} e^{-(x-d)/\lambda} & \text{for } x \geq d.
\end{cases}
\]

In Ref. [2], authors used the conventional approximation for the Townsend ionization coefficient of the form \( \alpha = A p \exp (-B p/E) \), with the effective field \( E \) calculated as average field over the cathode sheath, \( E = \varphi (d)/d \). In this work, we approximated \( \alpha \) by a more accurate estimation from Ref. [21]. As a decay constant \( \lambda \), we used an estimation proposed in [2],

\[
\lambda = \frac{\phi(d)/(pB) - d}{\alpha d},
\]

which makes it possible to approximate the decay scale \( \lambda \) in (9), given thickness \( d \) of the cathode sheath and voltage \( \phi (d) \). In this expression, parameter \( B \) is from the formula for the Townsend ionization coefficient \( \alpha \) and is equal to 180 V/(cm \cdot Torr) for an argon gas [22].

We incorporated ionization function \( S_{fast} \) defined by (9) into

(i) "simple" fluid model of glow discharge (section 2.1), where the plasma is composed of two species only, namely, the positive ions and electrons, and the ionization source function is

\[
S_e = S_i = S_{fast},
\]

(ii) "extended" fluid model of glow discharge (section 2.2), where we have added \( S_{fast} \) term in the right hand of equation (7) and the excitation term 0.5 \( S_{fast} \) in in the right hand of (8), respectively:

\[
S_e = S_i = S_{fast} + K_2 n_0 n_e + K_5 n_m n_e + K_6 n_m^2, \\
S_m = 0.5 S_{fast} + K_3 n_0 n_e - K_3 n_m n_e - K_5 n_m n_e - 2 K_6 n_m^2 - K_7 n_m.
\]

In the model (i), slow electron mobility and diffusion, \( \mu_e \) and \( D_e \), have been taken to be constants corresponding to those of the model (ii) corresponding to the temperature \( T_e = 1 \) eV.

In the near-cathode plasma of NG and FDS, the electric field is weak (and even may change a sign), so that the Joule heating in this region is also weak. Heating of the plasma (bulk) electrons is carried out by the Coulomb collisions with fast electrons. The corresponding term in the equation of electron energy balance can be estimated (see Refs. [23, 24] for details) by

\[
P_{fast} = \frac{1}{2} e^* S_{fast} \frac{\nu_{ee}}{\nu_{ee} + \delta \nu_{ea} + \nu_{df}},
\]
Present model:
Ext. fluid model:
S (9), \( \gamma = 0.01 (E/n) \)
\( \gamma = 0.6 \)
S from [20]
Hybrid model [5]:
S (9), model 2.
S (9), model 1.

Figure 2. Comparison with the hybrid model results from [5], for the set of conditions \( p = 133 \) Pa, \( V = 250 \) V, \( L = 1 \) cm, \( \gamma = 0.06 \). Spatial distributions of (a) electron and ion density, (b) electric field, (c) ionization source function, (d) electron temperature.

where \( \nu_{df} = 1/\tau_{df} = \Lambda^2/D_{ef} \), \( \Lambda \) is the characteric diffusive scale \( (R/2.4 \) for a cylinder), \( D_{ef} \) is the free diffusion coefficient of electrons. It is assumed that the electrons coming down from the inelastic region of EDF, uniformly fill in an energy range from 0 to \( \varepsilon^* \) (\( \varepsilon^* \) denotes the threshold energy for inelastic collisions) so that their average energy is \( 1/2 \varepsilon^* \). Thus, \( D_{ef}, \nu_{ea}, \) and \( \nu_{ee} \) are calculated for this value of energy (or temperature) of electrons [23, 24].

2.4. Boundary Conditions

Boundary condition for the positive ions, metastable atoms, and electron energy density at the anode and cathode are given as follows,

\[
\hat{n} \cdot \Gamma_i = 1/4v_i n_i + \alpha n_i \mu_i (\hat{n} \cdot \mathbf{E}),
\]

\[
\hat{n} \cdot \Gamma_m = 1/4v_m n_m,
\]

\[
\hat{n} \cdot \Gamma_e = 1/3 v_e n_e.
\]

Here, \( v_j = \sqrt{8k_B T_j/\pi m_j} \) \((j = e, i, m)\) denotes the thermal velocity, the flux density \( \Gamma \) is described by the equations (3) and (4), \( \hat{n} \) is the normal unit vector pointing towards the surface, and \( \alpha \) is a switching function (either 0 or 1) depending on positive ion drift direction at the surface: \( \alpha = 1 \) if \( (\hat{n} \cdot \mathbf{E}) > 0 \), and \( \alpha = 0 \) otherwise.

Boundary conditions for the electron density at the anode is

\[
\hat{n} \cdot \Gamma_e = 1/4 v_e n_e,
\]
Figure 3. Comparison with the hybrid model results from [5], for the set of conditions $p = 40$ Pa, $V = 441$ V, $L = 3$ cm, $\gamma = 0.033$. Spatial distributions of (a) electron and ion density, (b) electric field, (c) ionization source function, (d) electron temperature. "Star" in panel (a) indicates the measured electron density from [5].

and at the cathode

$$\mathbf{n} \cdot \mathbf{\Gamma}_e = 1/4 n_e n_i - \gamma \mathbf{n} \cdot \mathbf{\Gamma}_i,$$

where $\gamma$ is the secondary electron emission coefficient.

For the electric potential, we set $\phi = U_d$ at the anode and $\phi = 0$ at the cathode.

3. Modelling results
In order to demonstrate the performance of the model, first we carried out test simulations for the discharge conditions from [5]. Figures 2 and 3 compare spatial distributions of the discharge parameters obtained by the hybrid model from Ref. [5] with those obtained from the present model, for the two sets of conditions. The first set comprises $p = 133$ Pa, $V = 250$ V, $L = 1$ cm, $\gamma = 0.06$. For the second set, the parameters are $p = 40$ Pa, $V = 441$ V, $L = 3$ cm, $\gamma = 0.033$. Figures 2 and 3 contain (a) the distributions of the electron and ion densities, $n_e$ and $n_i$, (b) electric field magnitude $E$, (c) ionization source functions $S$, and (d) electron temperature, $T_e$. These figures illustrate also numerical results obtained by the "extended fluid" model (described in section 2.2), and the results obtained with the ionization function from Ref. [20] integrated into the "extended" fluid model.
As can be seen from Figs. 2 and 3, proposed model provides much better performance compared to the "extended fluid" model. Magnitudes and shapes of the charged particle densities (panels (a)) as well as the electric field (panels (b)) are close to those obtained from the hybrid model. Also, the electron temperature is not overestimated as in the case of the "extended fluid" model (panels (d)). Recall the fact that the strong overestimation of $T_e$ (and correspondingly the underestimation of $n_e$) is one of the main disadvantages of the fluid model, and attempts to improve it by taking into account non-Maxwellian EDF could lead to even worse results [25]. This is associated with the specific features of fluid description (more precise, the "extended" fluid description), in which the kinetic characteristics, specifically, the ionization rates are determined by the temperature (mean energy) of the electron ensemble. Within such a model, the electron gas in the plasma is heated by the heat flux $\Gamma_e$ from the cathode layer due to heat conduction rather than by a small group of fast electrons escaping from the layer. In a real situation, plasma electrons are heated by collisions with fast electrons, relative density of which is extremely low. Other sources of electron heating (such as Penning ionization, dissociative ionization in collisions of two excited particles, deexcitation by electron impact, etc.) here are also ineffective. Therefore, temperature of plasma electrons is uniformly distributed and low (no higher than several fractions of an electronvolt [26]).

As can be seen from Fig. 2, models with nonlocal ionization source, derived from the "simple" and "extended" fluid models of sections 2.1 and 2.2, practically coincide under the studied (short) discharge conditions, because the nonlocal ionization term dominates over other ionization processes involved, namely stepwise and Penning ionizations.

As always in models for the glow discharge, secondary emission coefficient $\gamma$ is one of the main sources of uncertainty. In order to demonstrate the effect of this parameter, Fig. 2 contains also numerical result obtained using the parameter $\gamma$ approximated by [27]

$$\gamma = 0.01 \left(\frac{E}{n}\right)^{0.6}_e,$$

where the reduced electric field is evaluated at the cathode, and given in units of kTd (1 kTd = $10^{-20}$ V cm$^2$). For the second reference conditions set, $\gamma$ determined by (16) appears to be very close to $\gamma = 0.033$ such that the numerical results obtained with these parameters practically coincide (in Fig. 3 we presented results for $\gamma = 0.033$ only).
Figure 5. Electron density at $x = 1.5$ cm from the cathode as a function of discharge voltage. $L = 3$ cm, $p = 40$ Pa, $\gamma = 0.033$. Figure also contains measured and computed data from [5].

Figure 4 compares measured volt-ampere characteristics (VAC) of Refs. [11, 28, 29] and VAC from the semi-analytical calculations of Ref. [2] with those obtained from the present model for $pL = 0.5$ cmTorr, with parameter $\gamma$ approximated by the equation (16) and one half of this $\gamma$, and with parameter $\lambda$ determined by (10) and by constant $\lambda = 0.1$ cm. It is seen that results of the proposed model are close to those obtained from the measurements and it provides much better performance compared to the "extended fluid" model.

Figure 5 plots the electron density at distance $x = 1.5$ cm from the cathode as function of the discharge voltage, for the discharge with $L = 3$ cm, $p = 40$ Pa, and $\gamma = 0.033$. This figure compares the present model results with measured data and data obtained from the hybrid model as well as from different fluid models of Ref. [5]. As can be seen from Fig. 5, present model more adequately predicts the charged particle densities than fluid models. It should be also noticed that version of the "extended fluid" model applied in this work demonstrates better performance than those from Ref. [5].

4. Conclusions
We proposed a simple hybrid model for a glow discharge, which incorporates nonlocal ionization by fast electrons into the fluid framework, and thereby overcomes the fundamental shortcomings of the fluid model. At the same time, proposed model is computationally much more efficient compared to the models involving Monte Carlo simulations. Calculations have been performed for an argon gas. Comparison with the experimental data as well as hybrid (particle) and fluid modelling results exhibits good applicability of the proposed model.

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