Simulation of negative corona discharge in atmospheric air: from mode of Trichel pulses to stationary discharge

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Abstract. The paper presents a 2D multi-fluid non-stationary model of a negative corona discharge in atmospheric-pressure air in the needle-to-plane diode. Discharges were simulated in gaps up to 1 cm with an applied voltage in the range of 8-100 kV. The simulation results demonstrate two stages of the discharge evolution: a pulsed-periodic stage called the Trichel pulses mode and a stationary glow discharge mode. The spatio-temporal distributions of the discharge plasma and electric field are shown in detail. Physical mechanism of Trichel pulses formation and transition to the stationary discharge are also revealed. The duration of the Trichel pulse mode gradually decreases with increasing of the applied voltage.

1. Introduction
Corona discharge in atmospheric-pressure air is a self-sustained low-energy discharge process occurring in a strong electric field near an electrode with a small radius of curvature. This phenomenon has permanently attracted interest of researchers [1, 2] and has received application in various technologies. The corona discharge can be divided into positive and negative polarities according to the polarity of the high-voltage electrode. A special attention is paid to the pulse-periodic (or Trichel pulses) mode of the negative corona discharge. Since Trichel reported this phenomenon in 1938 [3], a lot of research, including experiment and simulation, has been performed to make clear the physical mechanisms responsible for the pulse-periodic current mode. Loeb et al [4] found that the Trichel pulses occur only in electronegative gases. Later Akishev et al [5] have found that Trichel pulse sequence also occurs in non-electronegative gases such as pure nitrogen. However, there is no clear opinion on this issue at the moment. The experimental studies [6, 7] have shown that the first pulse was distinctly different from the subsequent pulses. The Trichel pulses also have been investigated by simulation. Morrow [8, 9] propose a one-dimensional model of negative corona discharge in air and oxygen. He believes that the secondary emission of electrons and photoionization process are the main factors affecting the formation of the pulse. Tran et al [10] and Sattari et al [11] have recently established the two-dimensional numerical model of negative corona discharge. On the other hand, researchers have focused on the mechanism of a transition from pulsed-periodic mode to stationary mode. Giao and Jordan [12] have investigated that the recombination and detachment rates of negative ions play a key role in removal of negative ions leading to the stationary mode. Some researchers have discussed the effect of gas heating on the transition mechanism. Chen et al [13] have proposed that gas heating decreases the gas density near the cathode so that the stationary mode is easy to achieve. However, Zhang et al [14] has established that the gas heating is not a dominant factor for the transition.
Despite numerous research works of the pulse-periodic mode of negative corona discharge and the transition to the stationary discharge, some explanations are still required. In this paper, we propose a multi-fluid model of the negative corona discharge describing the transition from the Trichel pulses mode to the stationary mode.

2. Theoretical model

To calculate the distributions of spatial characteristics of the non-stationary gas discharge, a theoretical model of corona discharge in atmospheric pressure air was formulated. The model is based on the hydrodynamic assumption, i.e. on the description of plasma evolution using the hydrodynamic equations. Electron component describes by the following system of continuity equations:

$$\frac{\partial n_e}{\partial t} + \nabla \cdot \Gamma_e = R_e,$$

$$\frac{\partial n_e}{\partial t} + \nabla \cdot \Gamma_e + E \cdot \Gamma_e = R_e,$$

where $n_e$ is electron density, $\Gamma_e$ is electron flux, $R_e$ is electron rate expression, $n_e = n_e^+ e$ is electron energy density, $e$ is mean electron energy, $\Gamma_e$ is electron energy flux, $E$ is electric field strength, $R_e$ is electron energy loss or gain due to inelastic collisions.

The hydrodynamic fluxes are defined using the drift-diffusion approximation as:

$$\Gamma_e = -\mu_e n_e E - D_e \nabla n_e, \quad \Gamma_e = -\mu_e n_e E - D_e \nabla n_e,$$

where $\mu_e$ and $D_e$ are electron mobility and diffusivity, $\mu_e$ and $D_e$ are electron energy mobility and diffusivity respectively. The transport coefficients have been obtained using the BOLSIG+ two-term Boltzmann equation solver [15] with the input cross-section data from [16].

The source coefficients in the equations (1) and (2) are determined by the plasma chemistry and can be written as:

$$R_e = \sum_{j=1}^{M} x_j k_j N_a n_e, \quad R_e = \sum_{j=1}^{P} x_j k_j N_a n_e \Delta \epsilon_j,$$

where $M$ is a number of reactions affecting generation and departure electron, $x_j$ is mole fraction of the target species for reaction $j$, $k_j$ is rate coefficient for reaction $j$, $N_a$ is the total neutral number density, $P$ is a number of inelastic electron-neutral reactions, $\Delta \epsilon_j$ is energy loss or gain of reaction $j$.

The heavy species describes by the following set of continuity equations ($k = 1...P$):

$$\rho \frac{\partial \omega_k}{\partial t} - \nabla \cdot j_k = R_k,$$

where $\rho$ is mixture density, $\omega_k$ is mass fraction of the $k$-th species, $j_k$ is a drift-diffusive flux vector, $R_k$ is rate expression for $k$ species.

The drift-diffusive flux vector is defined as:

$$j_k = \rho \omega_k \left[ D_{k,m} \left( \frac{\nabla \omega_k}{\omega_k} + \frac{\nabla M_n}{M_n} \right) - z_k \mu_{k,m} E \right],$$

where $D_{k,m}$ is the mixture averaged diffusion coefficient, $M_n$ is mean molar mass of mixture, $z_k$ is charge number for species $k$, $\mu_{k,m}$ is mixture averaged mobility for species $k$. The diffusion coefficients were computed according the paper [17].

The rate expression $R_k$ is determined by the stoichiometry of the system through the equation.
\[ R_k = \rho \sum_{j} v_{kj} \left( k_{t,j} \prod_{i=1}^{f} \omega^V_{ij} - k_{r,j} \prod_{i=1}^{f} \omega^V_{ij} \right) \]  

(7)

where \( N \) is a number of reactions, \( M_k \) is mass fraction of species \( k \), \( v_{kj} \) is stoichiometric matrix, \( k_{t,j} \) is rate coefficient for the \( j \)-th forward reaction, \( v^V_{kj} \) is stoichiometric matrix corresponding to forward reactions, \( k_{r,j} \) is rate coefficient for the \( j \)-th reverse reaction, \( v^V_{kj} \) is stoichiometric matrix corresponding to reverse reactions.

The equations for electrons (1) – (2) and heavy species (5) are coupled to the Poisson’s equation in order to take into the account the electric field self-consistently:

\[ \nabla \cdot E = \frac{e}{\epsilon_0} \left( \sum_k z_k \rho \omega_k - n_k \right), \quad E = -\nabla \varphi, \]  

(8)

where \( e \) is elementary charge, \( \epsilon_0 \) is vacuum permittivity, \( Q \) is a number of charged heavy species, \( \varphi \) is electrostatic potential.

The boundary condition for the Poisson’s equation on the anode is \( \varphi = 0 \), on the cathode surface is \( \varphi = U_0 \). The cathode potential \( U_0 \) is calculated by the following equation:

\[ U_0 = U_{\text{source}} - IR_b - RC_b \frac{dU_0}{dt}, \]  

(9)

where \( U_{\text{source}} \) is source voltage, \( R_b \) is ballast resistance, \( C_b \) is blocking capacitance. A discharge current \( I \) is defined as:

\[ I = \int \left[ \sum_{k=1}^{Q} n \cdot j_k + n \cdot \Gamma_e + n \cdot \left( \epsilon_0 \frac{\partial E}{\partial t} \right) \right] dS, \]  

(10)

A gas discharge diode includes a thin needle high-voltage electrode with a small radius of curvature \( r_{\text{curv}} \) and a plane anode at a distance \( d \) from the needle (figure 1). A computational domain is relatively wide so that the open boundaries do not affect the plasma processes at the needle tip.

![Figure 1. Scheme of gas discharge gap (computational domain 1-2-3-4-5, symmetry axis 1-2, anode 2-3, open boundaries 3-4-5, cathode 5-1).](image_url)
Table 1. A plasma-chemical reaction set in air$^a$.

| # | Reaction$^b$ | Rate coefficient$^{c,d}$ | Type of reaction |
|---|---|---|---|
| R1 | $e + M \rightarrow e + e + M^*$ | cross-section calculated from eEDF$^2$ | Impact ionization |
| R2 | $e + e + M^* \rightarrow e + M$ | $k_2 = 10^{-19} \left(300 / T_e\right)^{9/2}$ | e-i recombination |
| R3 | $O_2 + N_2^* \rightarrow N_2 + O_2^+$ | $k_3 = 6 \cdot 10^{-11}$ | Ion recharging |
| R4 | $e + N_2^* + M \rightarrow N_2 + M$ | $k_4 = 6 \cdot 10^{-29} \left(300 / T_e\right)^{3/2}$ | Three-body recombination |
| R5 | $e + O_2^* + M \rightarrow O_2 + M$ | $k_5 = 6 \cdot 10^{-29} \left(300 / T_e\right)^{3/2}$ | Three-body recombination |
| R6 | $e + O_2 + O_2 \rightarrow O_2 + O_2^*$ | $k_6 = 1.9 \cdot 10^{-30} \left(300 / T_e\right) \exp \left[\frac{7}{3} \left(1 - \frac{300}{T_e}\right)\right]$ | Electron attachment |
| R7 | $e + O_2 + N_2 \rightarrow N_2 + O_2^*$ | $k_7 = 8.5 \cdot 10^{-32} \left(300 / T_e\right)^2 \exp \left[5 \left(1 - \frac{300}{T_e}\right)\right]$ | Electron attachment |
| R8 | $e + O + O_2 \rightarrow O + O_2^*$ | $k_8 = 10^{-31}$ | Electron attachment |
| R9 | $O_2 + O_2 \rightarrow e + O_2 + O_2$ | $k_9 = 2.2 \cdot 10^{-18}$ | Detachment |
| R10 | $N_2 + O_2 \rightarrow e + O_2 + N_2$ | $k_{10} = 6 \cdot 10^{-19}$ | Detachment |
| R11 | $O_2 + M + O_2^* \rightarrow M + O_2^+$ | $k_{11} = 2.4 \cdot 10^{-30}$ | Production of $O_2^+$ |
| R12 | $O_2 + O_2^* \rightarrow 2O_2 + O_2$ | $k_{12} = 1.88 \cdot 10^{-13}$ | Ion recharging |
| R13 | $e + O_2^* \rightarrow O_2 + O_2$ | $k_{13} = 1.4 \cdot 10^{-6} \left(300 / T_e\right)^{1/2}$ | Dissociative recombination |
| R14 | $e + O_2^* \rightarrow O + O$ | $k_{14} = 2 \cdot 10^{-7} \left(300 / T_e\right)$ | Dissociative recombination |
| R15 | $e + N_2^* \rightarrow N + N$ | $k_{15} = 2.8 \cdot 10^{-7} \left(300 / T_e\right)^{1/2}$ | Dissociative recombination |
| R16 | $e + N_2 \rightarrow e + N + N$ | $k_{16} = 10^{-7} \left(T_e\text{[eV]}\right)^{-1.6} \exp\left(-9.8 / T_e\text{[eV]}\right)$ | Impact dissociation |
| R17 | $e + O_2 \rightarrow e + O + O$ | $k_{17} = 4.2 \cdot 10^{-6} \exp\left(-5.6 / T_e\text{[eV]}\right)$ | Impact dissociation |
| R18 | $O_2 + O_2^* \rightarrow 3O_2$ | $k_{18} = 10^{-7}$ | i-i recombination |
| R19 | $O_2 + O_2^* \rightarrow 2O_2$ | $k_{19} = 10^{-7}$ | i-i recombination |
where \( n \) is outward normal, \( v_{\text{th}} = \left( \frac{8k_T}{\pi m_e} \right)^{1/2} \) is thermal velocity, \( R_{\text{surf},i} = \sum q_i \) – surface rate expression, \( G \) is a number of surface reactions, \( q_i \) is surface reaction rate. \( \gamma_i \) is secondary emission coefficient from the \( i \)-th positive ion species, \( \Gamma_i \) is ion flux of the \( i \)-th positive ion species at the electrode surface, \( j_0 = 3.4 \times 10^{11} \, \text{A/cm}^2 \), \( \beta = 10 \) is roughness coefficient, \( B = 6.54 \times 10^8 \, \text{V/cm} \), \( \varepsilon_i \) is the mean energy of the \( i \)-th species of secondary electrons.

The boundary conditions on the open boundaries 3-4-5 can be written as:

\[
\mathbf{n} \cdot \mathbf{\Gamma}_e = 0, \quad \mathbf{n} \cdot \mathbf{\Gamma}_i = 0, \quad \mathbf{n} \cdot \mathbf{j}_i = 0, \quad \mathbf{n} \cdot \mathbf{E} = 0. \tag{14}
\]

The numerical solution of the gas discharge equations system (1), (2), (5) and (8) was performed using the nonstationary finite element method implemented in Plasma Module of COMSOL Multiphysics software. The simulation employed nearly 90 thousand triangle finite elements and 500 thousand degrees of freedom (DOF).

3. Numerical results

The simulation of the negative corona discharge in atmospheric pressure air was carried out under the following input parameters of the model: radius of curvature \( r_{\text{curv}} = 100 \, \mu \text{m} \), interelectrode distance \( d = 10 \, \text{mm} \), source voltage \( U_{\text{source}} = -8 \ldots -100 \, \text{kV} \), ballast resistance \( R_b = 1 \, \text{MOhm} \), blocking capacitance \( C_b = 100 \, \text{pF} \), gas temperature 300 K and uniform quasi-neutral initial distributions of the plasma components density. The calculation was conducted in a time range from 0 to 200 \( \mu \text{s} \) with a non-linear time step (from \( \approx 1 \, \text{ns} \) to resolve a current pulse to \( \approx 0.2 \, \mu \text{s} \)).

Figure 2 shows the current time profile throughout the time of interest. The evolution of corona discharge has two stages: a stage of Trichel pulses mode (figure 2 (a)) and a stable stage or glow discharge type (figure 2 (b)). The Trichel pulses have varying amplitude and repetition rate: the amplitude decreases whereas the repetition rate increases in time. The amplitude of the first pulse is several times larger than that of subsequent pulses. With increasing the applied voltage, the amplitude of the first pulse slightly increases, but that of subsequent pulses changes negligibly due to the current limitation by the space charge. The duration of Trichel pulses mode is determined by the rate of plasma propagation and the interelectrode distance.

Figure 2. Current time profile at \( U_{\text{source}} = -8 \, \text{kV} \): (a) Trichel pulses mode and (b) stationary discharge.
Figure 3. Distributions of the plasma components density (in cm\(^{-3}\)) and electric field strength (in kV/cm) during the second current pulse at different time points: (a), (b) – 20.0 µs (point a); (c), (d) – 21.2 µs (point b); (e), (f) – 21.5 µs (point c); (g), (h) – 22.3 µs (point d).

We believe that the reason of the pulse-periodic current mode is the presence of negative ions. As the plasma propagates, a spatial separation of charge occurs: a positive space charge consisting mainly
of $O_4^+$ is formed near the needle tip, a negative space charge consisting mainly of $O_2^-$ is formed a little further from the needle (figure 3 (a, b)). Production of electrons due to the ionization processes and field emission and their drifting away from the needle leads to the compensation of positive space charge (figure 3 (d)). At the same time the electrons attach to the molecules and form the negative space charge near the needle tip (figure 3 (c)). This leads to the current increase. Electric field is compressed near the tip (figure 3 (f)) and the negative ions drift away. Recombination of the high density ($\approx 10^{12}$ cm$^{-3}$) positive $O_4^+$ and negative ions also contributes to the ion-ion plasma neutralization. Hence the negative space charge leaves the region of a strong electric field (figure 3 (e)) and the current decreases. Electric field restores and conditions for a new current pulse are created (figure 3 (g, h)).

After the plasma has filled the diode and reached the anode, the negative corona discharge makes a smooth transition to the stationary mode. The Trichel pulse sequence builds up a plasma background leading to the formation of a plasma channel. The duration of the Trichel pulses mode and the channel formation time are determined by the applied voltage and are shown in table 2.

Table 2. A duration of the discharge evolution stages at different applied voltage.

| Applied voltage $U_{\text{source}}$ (kV) | Trichel mode duration (µs) | Channel formation time (µs) |
|----------------------------------------|---------------------------|-----------------------------|
| –8                                     | 80                        | 50                          |
| –15                                    | 25                        | 26                          |
| –30                                    | 7.8                       | 15.4                        |
| –50                                    | 4.0                       | 9.5                         |

4. Conclusion

A 2D hydrodynamic model of the negative corona discharge in atmospheric-pressure air is presented. Numerical results are demonstrated that the evolution of corona discharge at constant applied voltage includes a transition from the Trichel pulses mode to the stationary glow discharge. The pulse-periodic mode is caused by the presence of negative ions: the accumulated negative ions near the cathode can suppress the electric field. The results are also shown that the Trichel pulse sequence over time builds up a plasma background leading to the formation of a stationary discharge. The duration of the Trichel pulse mode gradually decreases with increasing of the applied voltage and this stage practically disappears at a voltage of 100 kV. We have been found a good agreement between the results of our modelling and the existing experimental data.

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