Simulation of high-pressure gas breakdown under conditions of spatially non-uniform initial ionization and temperature

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Abstract. The paper presents the results of numerical simulation of the extended atmospheric pressure discharge in configuration of the tip-to-plane diode. The simulation is based on a hydrodynamic model of a discharge plasma in a pure O₂ medium at low average electric field strengths ~ 10 kV·cm⁻¹. It was investigated how initial conditions, such as the presence of a weakly ionized plasma channel or a given temperature profile on the discharge axis, influence on the formation of a discharge structure at the initiation stage.

1. Introduction
It is known that at the initiation of breakdown in atmospheric pressure gas, under certain conditions, the area of channel germination takes on an elongated shape, as, for example, in the apocampic discharge [1]. The shape of the channel formed is simultaneously affected by many factors: the geometry of the electrodes and of the discharge chamber, composition of gas mixture and plasma-chemical processes, including photoionization [2], relaxing plasma remaining from the previous channel, etc.

In this paper, an attempt was made to reveal how the residual plasma from the previous voltage pulse between the electrodes may influences the nucleation of a channel in an oxygen environment. To this end, a model was built that allows one to take into account the main parameters of the relaxing plasma from a preliminary pulse, such as the concentration of charged particles and temperature, in a simple geometry tip-to-plane. To simplify the analysis, initial model profiles of plasma concentration and temperature were set.

2. Model
The simulation is based on a hydrodynamic model of discharge plasma in a pure O₂ medium at the pressure of 1 atm and the low average electric field strengths ~ 10 kV·cm⁻¹. Hydrodynamic equations were solved using the Plasma module of COMSOL Multiphysics 5.2 software.

Considered such reactions as ionization by electron impact with the formation of an O₂⁺ ion, attachment of electrons with the formation of an O₂⁻ ion, direct dissociation of the molecule with the formation of atomic oxygen, and ion-ion recombination: e + O₂ → 2e + O₂⁺, e + O₂ → O₂ + O₂⁻, e + O₂ → e + 2O, O₂⁺ + O₂⁻ + O₂ → 3O₂. Rate constant were taken from the reference [3] and other known sources.

The calculation was carried out for the configuration of the tip-to-plane diode in cylindrical symmetry (figure 1). A voltage pulse with an amplitude of 100 kV with a duration of 2.5 µs and a
leading front of 800 ns was applied to the electrodes with an interelectrode distance of 10 cm through the ballast resistance 10 kΩ.

![Figure 1. The computational domain configuration (h = 10 mm, L = 100 mm, d = 100 mm, r = 2 mm).]

In order to determine the effects on the initiation of a discharge of such factors as inhomogeneity of the initial concentration of charged particles and the presence of a temperature gradient, three variants of initial conditions were considered: 1) the initial concentration of electrons was $10^2$ cm$^{-3}$, the initial temperature of the medium was homogeneous and equal to $T_0 = 300$ K, 2) the initial electron concentration was set by a Gaussian function with a concentration in the center of the profile was equal to $10^{11}$ cm$^{-3}$ and characteristic spatial parameters $r_0 = 0.5$ mm and $z_0 = 47$ mm (figure 2), the initial medium temperature $T_0 = 300$ K, 3) the initial electron concentration was equal to $10^2$ cm$^{-3}$, the medium temperature was set Gaussian profile, with the maximum temperature 1000 K and with characteristic spatial parameters $r_0 = 1$ mm and $z_0 = 10$ mm (figure 3). For all three variants, the initial concentration of negative molecular ions was $9 \times 10^2$ cm$^{-3}$, and the initial concentration of positive molecular ions was found from the electroneutrality condition.

![Figure 2. Initial electron density profile (cm$^{-3}$).](image1)

![Figure 3. Temperature profile (K).](image2)

3. Results and Discussion

Simulations have shown that inhomogeneous initial conditions can change the shape of the plasma channel. Figure 4 shows concentration profiles at 250 ns from the moment the voltage pulse is applied. From a comparison of figure 4a and 4b, it can be seen that already at this stage the presence of pre-ionization increases the region of elevated plasma particle concentration near the cathode. Figure 4c shows that the presence of a narrow heated region leads to the rapid formation of a plasma in this region.
At a later stage with the expiration of 400 ns, the difference in the influence of the initial conditions on the channel shape becomes even more noticeable (figure 5). The widest channel is formed under homogeneous initial conditions, which corresponds to case a single pulse without pre-ionizations (figure 5a). The presence of a pre-ionized channel results in a smaller plasma spreading in the radial direction (figure 5b). Preheating leads to the greatest narrowing of the plasma channel (figure 5c). At the same time, the channel begins to expand and branch out approximately in the region of temperature drop in the initial profile (figure 3).

**Figure 4.** Spatial distribution of the $O_{2}^+$ number density (scale in cm$^{-3}$) for gas discharge (a) homogenous initial conditions, (b) with a Gaussian pre-ionization channel and (c) with a Gaussian preheated channel for the 250 ns time point.

**Figure 5.** Spatial distribution of the $O_{2}^+$ number density (scale in cm$^{-3}$) for gas discharge (a) homogenous initial conditions, (b) with a Gaussian pre-ionization channel and (c) with a Gaussian preheated channel for the 400 ns time point.

Accordingly, the presence of a preheated channel has the greatest effect on the narrowing of the breakdown channel in the initial stage. Undoubtedly, all these factors act together. And the process of channel formation is affected by other factors, the most important of which is plasma chemistry. Despite this, the proposed model allows to properly track major trends. To improve the understanding of the process of forming a breakdown channel, further complication of the model will be required by adding plasma-chemical reactions and complicating the discharge geometry. The results of the calculations make it possible to qualitatively explain how the relaxing plasma generated by the previous pulse can influence the process of development of the discharge when the next voltage pulse is applied. These results will be used later to construct qualitative models of repetitively pulsed discharges with complex spatial geometry, for example, the apocampic discharge [1].
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References
[1] Sosnin E A, Panarin V A, Skakun V S, Baksh E K and Tarasenko V F 2017 EPJ D 71 25
[2] Pancheshnyi S 2005 Plasma Sources Sci. Technol. 14 645
[3] He J and Zhang Y T 2012 Plasma Process. Polym. 9