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PIC-MCC method with finite element solver for Poisson equation used in simulation of the breakdown phase in dense plasma focus devices

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Abstract. Using PIC-MCC method for simulation of the breakdown of plasma focus device we obtained electron energy distribution function, spatial distributions of potential and charged particle densities. Studied is the first phase of the development of ionization process at pressures 133 – 931 Pa. Satisfactory agreement with experiment of the PF-1000 operation is observed for pressures in the range 665 – 931 Pa.

1. Introduction

Various theoretical models were created for simulating Dense Plasma Focus devices. Up to now the majority of those models were concentrated on modeling the second (acceleration) and the third (pinch) phases of the PF discharge while the initial formation of the current sheet during the breakdown phase was in some way neglected. It is well known that the efficient acceleration and formation of the pinch column requires homogeneity of the current layer. However in many cases filaments or spokes-like structures were observed in the ignition phase [1,2,3]. These structures might become frozen in the plasma. Then in front of the plasma layer magnetic stray fields born from the inhomogeneities can arise, which prevent the maximum compression of the plasma on the focus axes. Hence the breakdown and formation of the current sheath in the volume strongly influences the final focus phase. That is why a detailed description of this stage is necessary. In several papers the initial phase of the discharge was studied by hydrodynamic models [4-6]. In them Maxwell distribution of electron energy is assumed, but as it is shown in [7], during the first 15-20 ns after the device starts; the electrons do not have such a distribution. So a more accurate treatment of this problem is the stochastic one. The difficulties that arise when the initial phase of various fast discharges should be treated by a kinetic approach are substantial. Besides the space and time dependencies of the kinetic equation, a large number of particle interactions in the gas should be taken into account.

Only few such works exist in the literature. Kline and Siambis gave a kinetic description of the avalanche development [8]. Kunhardt et al. [9,10] investigated the stochastic development of electron avalanches and worked out their transition into streamers in nitrogen at a pressure of 1 ATM, comprising kinetic and hydrodynamic treatment. Slavin and Sopin [11] made a 1-D model of the fast ionization wave in a long cylindrical discharge at a very high rate (10¹³ V/s) of the voltage ramp. They divide the electron distribution into two parts – Maxwell bulk and fast electron group – and solve the
Boltzmann equation for the fast electrons. Starikovskaya and Starikovskii [12] gave a complete kinetic treatment of the fast ionization wave. Most of these works are dealing with nanosecond discharges, where the runaway electrons are playing quite an important role in the discharge development [13]. In the PF device the voltage increases linearly at a slower rate \(10^{11} \text{V/s}\); besides, PF geometry is quite complicated unlike those in works [8-13]. Therefore the results obtained for the nanosecond discharges are not applicable.

This paper continues the study of ionization growth in the breakdown of PF started in [7]. The difficulties, which we met in the previous work, stem from the specific spatial distribution of the charged particles and its effect on the electric field calculation. The electric field was calculated by a finite difference method with a limited value of spatial discretisation ratio. At a certain moment the spatial step becomes comparable with the Debye radius. Due to this fact spurious electric fields appear in the simulation about 16-17 nanoseconds after the beginning. Now the finite difference method is replaced with a finite element method with an adaptive mesh, which adjusts to the charged particle spatial distribution peculiarity. This method allows us in a reasonable computational time to obtain the discharge evolution for up to 20-30 ns. Here we also use a more complete database for the collision cross sections.

Practically the breakdown itself can be divided into two stages. In the first stage an ionization of the neutral gas occurred up to charge particle densities \(10^{14}-10^{15} \text{m}^{-3}\), while during the second stage a substantial rise of the charged particles density and respectively the discharge current is observed and current sheet is formed. This study is dedicated to the first stage of the breakdown.

2. Description of the model

Figure 1 gives a schematic representation of the Plasma Focus coaxial electrodes in the area where the breakdown occurs.

![Figure 1. Cross Section of the Plasma Focus Device geometry.](image)

The concrete geometry parameters used in our simulation are: \(R_k = 0.075 \text{m}\), \(R_a = 0.05 \text{m}\), \(R_d = 0.045 \text{m}\), \(Z_1 = 0.10 \text{m}\), \(Z_2 = 0.15 \text{m}\). The initial number of charged particles is chosen here to be 2000. This corresponds roughly to density equal to \(1.4 \times 10^6 \text{m}^{-3}\). We are considering only 1.5 liters from the whole volume of PF – 1000, which are important for the breakdown.

The code is based on a Particle In Cell – Monte Carlo Collisions (PIC-MCC) method. It consists of four modules (Figure 2) each one described bellow.

![Figure 2. Scheme of numerical method.](image)
2.1. In the “Particle Movement” module we solve equations of motion of charged particles. If a particle leaves the volume we generate a collision with boundary. The particles are absorbed by the dielectric and form a surface charge. The electrons are reflected by the cathode, and the ions hitting the cathode eject electrons with a ratio $\gamma = 0.15$.

2.2. The “Collisions procedure” generates collision events by Monte Carlo method using the cross sections of each scattering process [14, 15]. The double differential cross sections for the elastic scattering and ionization are taken from works [16, 17]. The collisions used are shown in the Table 1.

Table 1. List of the processes used in the model.

| Scattering process            | Reaction                                      |
|-------------------------------|-----------------------------------------------|
| Elastic electron collision    | $e + H_2 \rightarrow e + H_2$                 |
| Elastic ion collision         | $p + H_2 \rightarrow p + H_2$                 |
| Ionization                    | $e + H_2 \rightarrow 2e + H_2^+$              |
| Rotational excitation         | $e + H_2 \left( X^1\Sigma_g^+, v = 0, J = 0 \right) \rightarrow e + H_2 \left( X^1\Sigma_g^+, v = 0, J = 2 \right)$ |
| Rotational excitation         | $e + H_2 \left( X^1\Sigma_g^+, v = 0, J = 1 \right) \rightarrow e + H_2 \left( X^1\Sigma_g^+, v = 0, J = 3 \right)$ |
| Vibration excitation          | $e + H_2 \left( X^1\Sigma_g^+, v = 0 \right) \rightarrow e + H_2 \left( X^1\Sigma_g^+, v = 1, 2, 3 \right)$ |
| Electronic excitation $b^3\Sigma_u$ | $e + H_2 \left( X^1\Sigma_g^+ \right) \rightarrow e + H_2 \left( b^3\Sigma_u \right)$ |
| Electronic excitation $a^3\Sigma_g$ | $e + H_2 \left( X^1\Sigma_g^+ \right) \rightarrow e + H_2 \left( a^3\Sigma_g \right)$ |
| Electronic excitation $D^3\Pi_u$ | $e + H_2 \left( X^1\Sigma_g^+ \right) \rightarrow e + H_2 \left( D^3\Pi_u \right)$ |
| Electronic excitation $B^1\Sigma_u$ | $e + H_2 \left( X^1\Sigma_g^+ \right) \rightarrow e + H_2 \left( B^1\Sigma_u \right)$ |
| Electronic excitation $C^1\Pi_u$ | $e + H_2 \left( X^1\Sigma_g^+ \right) \rightarrow e + H_2 \left( C^1\Pi_u \right)$ |
| Electronic excitation $C^3\Pi_u$ | $e + H_2 \left( X^1\Sigma_g^+ \right) \rightarrow e + H_2 \left( C^3\Pi_u \right)$ |
| Sum of excitations to Rydberg levels | $e + H_2 \left( X^1\Sigma_g^+ \right) \rightarrow e + H_2 \left( \text{Rydberg} \right)$ |

2.3. In the “Weighting” module the PIC (particle in cell) scheme is used to obtain densities of the charged particles. The weighting procedure is based on the standard Matlab function – “Nearest triangle search”. It is optimized for faster weighting while sub-cycling for mesh refinement.

2.4. The “Field” module calculates the electric field by solving the Poisson equation. More accurate treatment is to solve Maxwell equation, and to take into account induced magnetic field. In fact the induced magnetic field is not negligible, because of the very fast rising of the electric field (anode potential increases linearly with a rate of $2 \times 10^{11}$ V/s). Probably the effect of magnetic field will decrease the mobility of the charged particles and correspondingly will decrease breakdown pressure. But this will complicate significantly the current model. We use the “pde” toolbox of Matlab program for solving the Poisson equation on a triangular mesh with a finite element method (FEM). The potential comprises the applied external field, the volume charge and the surface charge appearing from the electrons and ions generated in the vessel.

3. Results and discussion
After switching on the external field the initial electrons are accelerated and start to excite and ionize the hydrogen molecules. The exponential growth of charged particle number becomes apparent after about 5-6 ns from the beginning (see Figure 3). Depending on pressure the electron density have completely different behavior. At 133 Pa the electrons rapidly increase their energy and in the time interval 10-13 ns leave the volume without substantial ionization of the gas. At gas pressure of 399 Pa the electron density increases up to $2 \times 10^{12} \text{ m}^{-3}$ and at t=20 ns starts decreasing. It is connected with the high average energy of electrons (up to 95 eV). At that moment more than 13% of electrons at t=19 ns at this pressure have energy higher than 200 eV. The regimes at 665 and 930 Pa the electron density reaches $3 \times 10^{15} \text{ m}^{-3}$ at the end of the time interval studied in this work. In both curves we have a decrease of the average electron energy after t=17 ns connected with decreasing of the field just in front of insulator and anode due to substantial volume charge appeared. This can be seen on Figure 5 representing the potential distribution.

**Figure 3.** Average electron density at different pressures.  
**Figure 4.** Average energy of the electron ensemble at different pressures.  
**Figure 5.** Electric potential at pressure 665 Pa. The numbers on equipotential lines are in volts.
Figure 6 shows the spatial distribution of the electron density. It gives quite clear picture of the development of the process. Up to 10 ns electrons are generated and remain near the contacting point between the dielectric and cathode (between $Z = 0 - 0.01$ m) due to the strong electric field there. Afterwards they leave the volume and another group of electrons form a thin layer in front of the dielectric and anode. They are kept in the potential “well”, where the field is low. Due to the high frequency of electron-molecule interactions (elastic and mainly inelastic) the average energy of the electrons decreases and the energy distribution function becomes close to Maxwellian (Figure 7). It is seen from this picture that at $t=17$ ns the EEDF has much more electrons with energy above 200 eV compared to Maxwellian and respectively a deficiency of electrons at 80 - 100 eV, where energy losses are maximal. At $t=22$ ns the electron distribution function becomes close to the equilibrium distribution and the ionization rate begins to decrease.
4. Conclusion
PIC-MCC method allows us to obtain clearer picture of the preionization process in PF-1000. We studied the development of breakdown during the first 22 ns after switching on the discharge for pressures between 133 and 930 Pa. Between 665 and 930 Pa the results are in agreement with the experimental operation PF-1000 [18]. For pressures in the range of 133 – 399 Pa additional mechanisms should be incorporated in the model in order to obtain results closer to the experiment.

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